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GEMA3D – landscape modelling for dose assessments

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This report concerns a study which has been conducted for the Swedish Radiation Safety Authority, SSM. The conclusions and viewpoints presented in the report are those of the author/authors and do not necessarily coincide with those of the SSM.

SSM Perspective

Background

Post-closure safety assessments for nuclear waste repositories involve radioecological modelling for an underground source term. Following several decades of research and development, the Swedish Nuclear Waste Management Company (SKB) is approaching a phase of license application. According to SKB's plans, an application to construct a geological repository will be submitted by the end of 2010. The application will be supported by a post-closure safety assessment. In order to prepare for the review of the oncoming license application the Swedish Radiation Safety Authority (SSM), has performed research and development projects in the area of performance assessment (PA) modelling during recent years. Independent modelling teams have been established, including both "in house" as well as consultant's competences. Aleksandria Sciences undertaken research and development for the Swedish regulatory authorities over many years. This has included the development of approaches and models for consequence analysis (dose assessment) that can be used to support the review of submissions from SKB.

Objectives of the project

SSM held a workshop at Rånäs Castle from 18-20 February 2009 to discuss the status of Consequence Analysis capabilities and to plan for preparatory work in the current year. Out of this meeting and subsequent discussions, four areas were identified where further research during 2009 would be beneficial:

1. further development of a simplified general ecosystem modelling approach to cover all the ecosystems, like stream, lake, wetland and forest;
2. a study of the model sensitivities of a small system with various ecosystems due to different combinations by introducing the release to different ecosystems as well as taking into account the chemical zonation in model descriptions;
3. implementation of all the developed models in the numerical software, Ecolego. This report documents the research that was undertaken.

Project information

Project manager: Shulan Xu
Project reference: SSM 2009/1217
Project number: 1648

Abstract

Concerns have been raised about SKB's interpretation of landscape objects in their radiological assessment models, specifically in relation to the size of the objects represented – leading to excessive volumetric dilution – and to the interpretation of local hydrology – leading to non-conservative hydrologic dilution. Developed from the Generic Ecosystem Modelling Approach, GEMA3D is an attempt to address these issues in a simple radiological assessment landscape model.

In GEMA3D landscape features are model led as *landscape elements* (lels) based on a three compartment structure which is able to represent both terrestrial and aquatic lels. The area of the lels can be chosen to coincide with the bedrock fracture from which radionuclides are assumed to be released and the dispersion of radionuclides through out the landscape can be traced.

Result indicate that released contaminants remain localised close to the release location and follow the main flow axis of the surface drainage system. This is true even for relatively weakly sorbing species. An interpretation of the size of landscape elements suitable to represent dilution in the biosphere for radiological assessment purposes is suggested, though the concept remains flexible. For reference purposes an agricultural area of one hectare is the baseline.

The Quaternary deposits (QD) at the Forsmark site are only a few metres thick above the crystalline bedrock in which the planned repository for spent fuel will be constructed. The biosphere model is assumed to be the upper one metre of the QD. A further model has been implemented for advective – dispersive transport in the deeper QD. The effects of chemical zonation have been briefly investigated. The results confirm the importance of retention close to the release point from the bedrock and clearly indicate that there is a need for a better description of the hydrology of the QD on the spatial scales relevant to the lels required for radiological assessments.

Content

1 INTRODUCTION

Biosphere models for the assessment of radiological consequences of disposals of radioactive waste have tended to be simple and straightforward in conception. There has been much development over the years (BIOMOVS, 1993; BIOMOVS II, 1996; IAEA, 2003), and much discussion (cf. Bioprota, 2009). In the main, however, the structural elements of biosphere models have remained fairly constant over the decades with vertical transport in the soil column and accumulation in water bodies being the main focus for the representation of the near surface environment.

As SKB approach the submission of a site license application and the state of knowledge about the landscape near to the proposed disposal facility has increased, recent dose assessments have involved the development of "landscape models". In SR-Can (SKB, 2006a) the landscape comprised a system of linked compartment models, each representing the state of a "landscape object" as a function of time. The extent of the landscape was defined by the ensemble of possible release locations in the landscape realised by the mapping of canister positions in the repository to the potential outflow locations at the top of the bedrock.

For each individual landscape object (defined by SKB in terms of ecosystem within a catchment or basin on the basis of local topography) the compartment structure remained rather simplistic[1] and the flow systems poorly characterised. Indeed, these were the findings of the review carried out by Xu *et al*. (2008). The SSI (SSM) dose assessment model GEMA (Kłos, 2008a; 2008b) is somewhat more sophisticated, emphasising the potential for accumulation in surface systems. By including a representation of the surface drainage network the importance of dilution within the catchment was also indicated. One key difference between the SR-Can models of biosphere objects and the GEMA models was that the GEMA representations identified several sub-objects within the boundaries identified as a single large object in the SKB landscape. Results show that for even quite low k_d values, significant radionuclide retention close to the release point can be expected.

A further result from Xu *et al*. (2008) concerned the distribution of radionuclides in the Quaternary Deposits (QD) which make up the top few metres of the Swedish landscape. Analysis in SR-Can was on the basis of release *points* but Xu *et al.* showed that release from a fracture would expect to be distributed over an extended distance in the longitudinal direction and that spreading in the QD would at a transverse component. The extent of the release footprint in the QD would be expected to be around 1500 m long and 15 m wide, rather than the single point source at the base of the QD.

A new modelling approach (GEMA3D) has consequently been developed in which submodels based on simplified GEMA structural elements have been linked together in a network which represents the landscape as a set of "landscape elements" ("lels") each comprising three compartments. This documents sets out the basic details of a landscape model using GEMA3D and also includes an investigation of transport through the deeper QD.

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[1] It is expected that a far greater degree of model identification, justification and description will be forthcoming in dose modelling for SR-Site.

2 BIOSPHERE MODELLING FOR PERFORMANCE ASSESSMENT

2.1 Landscape objects in future Swedish biospheres

Forsmark is the site of the low- and intermediate level disposal facility SFR-1. SKB have also selected Forsmark as the location for their planned deep repository for spent fuel. The landscape around Forsmark is therefore of primary interest. It is, however, broadly representative of other parts of central and southern Sweden as well as parts of Finland.

The main features are, low relief, a mixture of lakes, wetlands and forests with agricultural potential if required, though there has been a decrease of agricultural land usage over the past century or so. The site is currently on the Baltic coast but the rapid rate of isostatic land rise (6 mm a^{-1}) means that a large areas currently beneath the Öregrundsgrepen will emerge and be transformed from coastal to terrestrial ecosystems. It is in this area that potential releases from the spent-fuel repository are anticipated. The terrestrial ecosystems to the south-west of the current coastline give a good indication of the surface environment to be expected over the next ten to twenty thousand years.

Topography is assumed to have the largest influence on future landscape. SKB have identified numerous basins from the topographic map of the bed of the Öregrundsgrepen and these will form future catchments. There will be some infilling of deeper parts of these during the evolution from marine to lacustrine and wetland periods. Significant accumulations of highly organic sediments will fill the depressions to form areas of wetlands which could be drained for future agricultural usage. According to the latest models of the area the typical depth of the QD would then be around 3 m (Lindborg, 2008). The wetland areas would not occupy the full extent of the basins/catchments but, having formed in the lower parts of the catchment, these would coincide with the fracture map and so be the locations of potential future releases.

2.2 Treatment in previous assessments

In earlier assessments – both SR-Can (SKB, 2006a) and the recent SAR-08 assessment for the SFR-1 repository (Bergström *et al.*, 2008), SKB have identified landscape objects as the entirety of the lake/wetland area. SSM modelling and reviews (Kłos, 2008b, Kłos and Shaw (2008), Kłos, 2009) have indicated that this is not necessarily the appropriate interpretation of *limiting* landscape objects in the future biosphere – i.e., those for which it is reasonable to expect that doses could occur should the release coincide with them and for which calculated doses would be at the higher end of the consequence scale.

SKB have concentrated on natural systems bays, lakes, wetlands and forests as these – in the present day – cover the greater part of the model area and while they also consider agricultural lands these are not always integrated into the assessment as compellingly as the other ecosystem types. One reason for this appears to be the use of carbon productivity as the determinant of landscape object size. Productivity of most of the ecosystems is low - Table 2-1. A large area (with implicit large dilution) is required to support even small human populations. However, the

Table 2-1. Productivity and supportable population for different ecosystem types. (Figures taken from Bergström et al., 2008, assuming a human adult requirement of 110 kg of carbon annually).

		ecosystem			
		agriculture	forest/mire	lakes	sea
Net C production	kgC m^{-2} a^{-1}	1.30E-01	3.00E-04	9.00E-04	5.30E-03
sup. pop dens	person m^{-2}	1.18E-03	2.73E-06	8.18E-06	4.82E-05
Min. area for 10 adults	m^2	8.47E+03	3.66E+06	1.22E+06	2.07E+05
Ratio	agriculture/ ecosystem	1	433	144	25

supportable population density of *agricultural land* is much higher, more than four hundred and thirty times higher than forests and wetlands. These figures indicate that the main focus of attention in the dose assessment should be agricultural systems, particularly in confined areas which could receive a source of contaminants from the fractured bedrock and which have limited dilution but which are large enough to support a population of a few tens of adults.

Based on the carbon productivity figure from Bergström *et al.*, which assumes all carbon production is consumed with no wastage or recycling, the minimum area of forest or mire required to support a population of ten adults would be more than three and half square kilometres.

For agricultural land an area of around 10^4 m^2 would be sufficient. It is acknowledged that the yield of crops and livestock is somewhat variable however. The productivity figures need for Sweden should be reviewed to obtain a better estimate of the size of representative landscape elements. In SR-Can and SAR-08 SKB's focus was on natural ecosystems and consequently the size of landscape objects was typically of the order of several million square metres.

For reasons of local concentration of contaminates, the primary focus of the GEMA3D model is the terrestrial landscape, particularly agricultural systems. Lakes are included as part of the landscape and bays and seas can equally be modelled, as required. It is anticipated, however, that agricultural objects are likely to be the limiting objects in any assessment dose modelling for SR-Site.

2.3 The GEMA3D concept

In the original generic ecosystem modelling approach (GEMA) concept (Kłos, 2008a) formed landscape models on an interpretation of catchments and sub-catchments in the surface drainage system. The fluxes of water and solid material between the different ecosystem models provided the dynamics of contaminant transport. Here the size of the landscape element – "lel" - is defined in terms of potential dispersion in the QD geology and a consideration of the size of the potentially exposed group.

From the above discussion it is apparent that a compartment area of 10^4 m^2 is a suitable size for usage in dose assessments. It could be argued that 10^3 m^2 – for a single adult could be used but the factor of ten greater area allows for implicit mixing of foodstuffs from different parts of the agricultural system. A set of landscape elements of these dimensions can be formulated to represent larger scale ecosystems (forests, mire, lakes and bays) as required. By modelling landscape feature as a set of landscape elements (lels) comprising vertical transport and horizontal movement between lels a comprehensive representation of the *contaminated* landscape can be constructed as a three dimensional model - this GEMA3D[2]. The method also provides for better integration with the geosphere-biosphere interface.

A generic arrangement is shown in Figure 2-1. Contaminant transport is determined by the

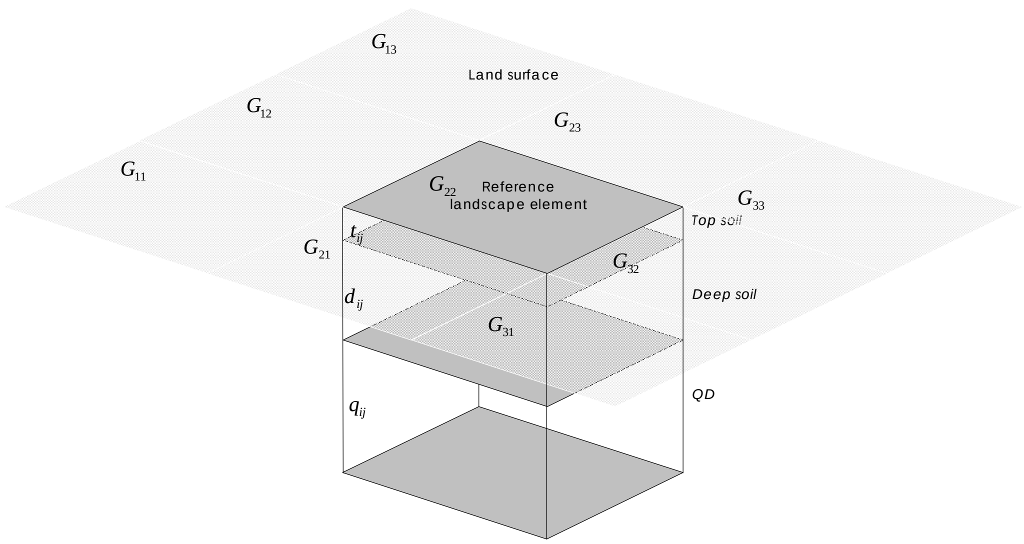

Figure 2-1. Generic arrangement of landscape elements (lels) in GEMA3D landscape model. Compartments in each lel are t- (top soil or water column), d- (deep soil or bed sediment) and q- (unmodified Quaternary deposits).

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2 A developed version which features an evolving system would be four dimensional and known as GEMA4D.

exchange of water and solid material between the compartments of the model. Diffusive processes can also be included though these are expected to be of little importance in the dynamic near surface environment. Within each lel water and solid fluxes may enter and exit to adjacent elements. As well as contaminated fluxes, uncontaminated material may also enter the lel as part of the overall mass balance of the system. Diffusive processes can also be represented though these processes are of much less significance than advective processes, especially in the upper part of the QD. In the deeper QD a finer spatial resolution is required than is the case in soils. This is discussed further in the following section and in detail in Chapter 5.

2.4 Radionuclide releases and spatial resolution of the lels

A prototype of the GEMA3D concept featuring nine lels arranged in the pattern shown in Figure 2-1 confirmed that diffusive fluxes are of minimal importance and so can be neglected in horizontal transport. This is a weakly conservative assumption in the there is less loss from contaminated lels than might be the case in reality. The prototype also confirmed that the lel receiving the input from the geosphere would be likely to be the one in which the maximum consequences would arise, on the spatial scale assumed in these models. There were situations in which activity flowing downstream, in an aquifer, along drainage system might give higher consequences downstream, were irrigation downstream to be a feature of the system. The prototype assumed a point source input to the base of the QD with rapid mixing implicit in the compartmental approach.

Following the modelling reported by Xu *et al.* (2008) on the likely surface footprint of a release to the base of the QD along a fracture the point-source interpretation of the release has been replaced by the following interpretation, specific to the crystalline bedrock beneath a shallow QD layer typical of Scandinavian conditions.

Fractures carry groundwater from the bedrock to the surface. The fractures manifest themselves as lineaments extend over hundreds of meters. Xu *et al.* showed that longitudinal dispersion along the fracture would amount to around 1500 m. The transverse extent of the plume is somewhat more speculative. The width is dependent on depth of the QD. A value of 15 m is quoted by Xu *et al.* for a QD thickness of 6 m. In the Scandinavian landscape fractures coincide with low points in the topography and are associated with lakes, wetlands and to some extent streams[3]. Whatever the width assumed it is likely that the highest concentrations in the surface soils would be within a few metres of any drainage system.

Calculating doses from such a narrow strip of land presents some difficulties. To maximise dose it could be assumed that cultivation along the highest contaminant concentration is consumed by a single critical group, however, such a pattern of behaviour is not seen in the historical record and is certainly not the practice today. Instead the assumption in GEMA3D is that a landscape element 100×100 m^2 (1 hectare) is the terrestrial element with a narrower and longer stream

[3] A distinction may be made between natural streams and managed drainage ditches and managed water courses.

element. As noted above, the 10^4 m^2 area is sufficient for the needs of a few adults, under agricultural cultivation. Assuming a wider area of land means that there is an implicit mixing between the most highly contaminated foodstuffs grown in the highest soil concentrations with the less highly contaminated soils further from the stream.

Furthermore, the nature of agricultural land is such that it is not natural. Agricultural areas in the Scandinavian landscape are often found on highly organic soils formed by in-filled lakes which have become wetlands but which have subsequently been deliberately drained. The drainage system is emplaced to suit the farmer and my not follow the bedrock fracture. Release to the base of the QD may therefore occur anywhere within the lel and is not constrained to follow the stream.

In the following section the key features, events and processes in the Scandinavian biosphere are outlined and the basic structure of a GEMA3D lel defined.

3 SYSTEM IDENTIFICATION AND DEFINITION

3.1 The GEMA3D landscape element

In the transport and accumulation model terrestrial elements comprise soils, including the rooting zone and sub-soils. Beneath the subsoil is a layer of largely unmodified Quaternary material within which there may be some water movement, depending on local hydrology. The characteristics of each type of soil/QD are influenced by the ecosystem type. Relevant characteristics are horizon thickness (depth) porosity, moisture content and local hydrogeochemistry (expressed as a radionuclide specific k_d-value). There are also suspended solid content of porewater and the density of the solid material.

Parameters defining water and solid material fluxes within the element are also specified: precipitation, ETp, capillary rise, biomass movements and deposition. Also relevant are the external sources of water and solid material – inflows from subsurface flows (aquifer) or run-off from adjacent (uncontaminated) catchment landscape elements. Inflows of solids with water (as suspended sediment) may be accounted for as well as regions of solid deposition. Outflows of water and solids are accounted for by mass conservation and balance may also be used to determine internal fluxes.

The area of the terrestrial compartment is set to the default area of the landscape model – 10^4 m^2 as noted in the preceding section – although each lel can be assigned its own specific value as required.

Aquatic lels are characterised in the same way as terrestrial elements with the difference that the upper compartment is the water column and the “thickness” is the depth of the water rather than the thickness of the top soil compartment. A sediment layer is anticipated between the water column and the QD compartment. Processes leading to water and solid material transfers are characterised in a similar way to those in the terrestrial compartment.

Areas of aquatic lels are not necessarily fixed to the default landscape resolution. A lake may be represented by a number of lels (to allow for local accumulations in those lels receiving the release rather than assuming a large object with corresponding dilution). Streams are, by their nature, long and thin. The length and width of a stream lel are defined and these together define the area of the overall landscape element.

Representation of contaminant transport in the lel requires that fluxes of water and solid material are included as input parameters for each lel. This includes internal fluxes between the compartments of the lel and sources and losses to and from the lel to other lels, including uncontaminated parts of the landscape which contribute only diluting fluxes but which must be included to account for mass balance.

GEMA3D is primarily a model of the upper part of the QD. Typically in the Forsmark context this is around one metre as it is in this region that the major water fluxes (principally of meteoric origin flow.

3.2 Deep Quaternary deposits

The thickness of the QD above the bedrock varies from very shallow superficial soils covering outcrops of bedrock to several metres in basins where there has been a greater accumulation of solid material in, first, bays, then lakes and wetland. Often these more recent deposits overlay glacial clays and tills. These depressions in the landscape are associated with the surface expression of the fracture network and correspond to locations of potential release in groundwater discharge.

Release from fractures into the upper model can be a dynamic process, depending on the time of the release. Potentially a chronic release could occur to increasing accumulations of lake bed sediments and thereby spread over the full thickness of the sediment. Alternatively the release could occur to the base of a few metres of tightly packed, organic rich sediment with little water movement. Diffusive spreading in the bed sediment layers would then be expected. As the overall water flux through the sediment is likely to be small compared with horizontal fluxes in the water column and the upper parts of the QD column under agricultural conditions, an advective dispersion “transport block” has been implemented as part of the model.

For this model a small water flux is assumed to enter the base of the QD column, discharging at the top of the column. Diffusion takes place through out the column. A compartment model is used and the column is subdivided into a number of layers, the number dependent on the particular problem. The parameters characterising the column are the chemistry – k_d value, the porosity and the density of the QD material. In principle, several of these blocks can be combined to represent varying properties along the QD column. A model for transport in the deeper QD is discussed in Section 5 of this report.

3.3 Implementation of landscape element models

GEMA3D is a compartment model. The implementation here is made using the Ecolego modelling tool produced by Facilia AB, Bromma, Sweden. Contaminant transport between compartments *i* and *j* in the network is represented by fractional transfer rates with the generic form

$$\lambda_{ij} = \frac{F_{ij} + k_i M_{ij}}{\left(\theta_i + (1-\varepsilon_i)\rho_i k_i\right)V_i} \ \mathrm{a}^{-1} \tag{3.1}$$

where:

V_i	[m^3]	is the volume of compartment *i*,
ε_i	[-]	is the porosity of the compartment,
θ_i	[-]	is the volumetric moisture content,

ρ_i [kg m^{-3}] is the solid material density, and

k_i [m^3 kg^{-1}] is the k_d of the contaminant in compartment i.

The drivers of the transport and the water (F_{ij} [m^3 a^{-1}]) and solid material (M_{ij} [kg a^{-1}]) fluxes between compartment i and j. n practice these are determined on the basis of local characteristics.

The implementation in Ecolego, of the model of the example system described in the following Section, is described in Appendix A and Appendix B discusses the detailed modelling of the QD column.

4 IMPLEMENTATION OF GEMA3D

4.1 Example system

The system implemented as a GEMA3D model here is used to illustrate features of the modelling approach. It is based on an interpretation of landscape objects anticipated at Forsmark under future conditions where land rise has exposed areas of land to the northeast of today's coastline. It is not intended to be a definitive radiological assessment model since there are many details in the Forsmark site descriptive model which need to be better integrated. In particular the hydrology under the lake features an idealised aquifer which is unlikely to occur in Forsmark lakes. However, the interpretation of drained agricultural systems is believed to be representative of practical farming conditions in similar landscapes.

A landscape feature from the future Forsmark landscape is used to illustrate GEMA3D. The feature in question is identified in SR-Can as Object 11 (and "the SAFE basin" in SAR-08: Bergström *et al*., 2008). The basin is shown in Figure 4-1 at after land rise of 15 m, when the Baltic coast of the Öregrundsgrepen, which lies some 500 m to the North, at the closest point. The landscape object at the centre of the basin (identified as FS1:05 by Kłos, 2008a) is the lowest lying part of Basin 11 and is expected to undergo a lake → wetland/forest transition over the next few thousand years. The map shows the object comprises a large number of 10^4 m^2 lels.

Although the present day landscape has only a small proportion devoted to agriculture, the needs of future societies for food production cannot be assumed to match those of today and it is reasonable to assume that the area defined by the object could, at some future time, be used, at least in part, for agricultural purposes. Devoted entirely to agricultural production the area could provide for over 1400 adults and each agricultural lel within the FS 1:05 object could support a few adults. In contrast only three or ten adults could be supported by the objects as lake or wetland respectively.

The definition of the system therefore requires some indication of the nature of the geosphere-biosphere interface for this landscape object. Future accumulations of contaminants within the QD of FS1:05 depend on the input of contaminated groundwater from the bedrock reaching the surface via fractures. Figure 4-2 is a map of the object with the lineaments indicated (SKB, private communication). It is expected that circumstances are possible in which there could be release to the QD at the base of the object. As noted in the introduction the plume from the bedrock might be expected to be around 1500 m in length and so would affect up to 15 of the lels in the object. The remainder would remain uncontaminated[4].

During periods when the object is a lake there would be little contaminant accumulation in QD sediments on top of the bedrock. With progressive sedimentation as the lake matures to a wetland there might be greater accumulations of contaminants in the QD. However, it is the chronic release to the QD beneath the wetland, with subsequent transformation (by human action) to agricultural land that is of primary concern here.

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[4] It is possible that the centroid of the plume might migrate along the fracture during the period of release. For present purposes it is sufficient to note that several lels would be affected.

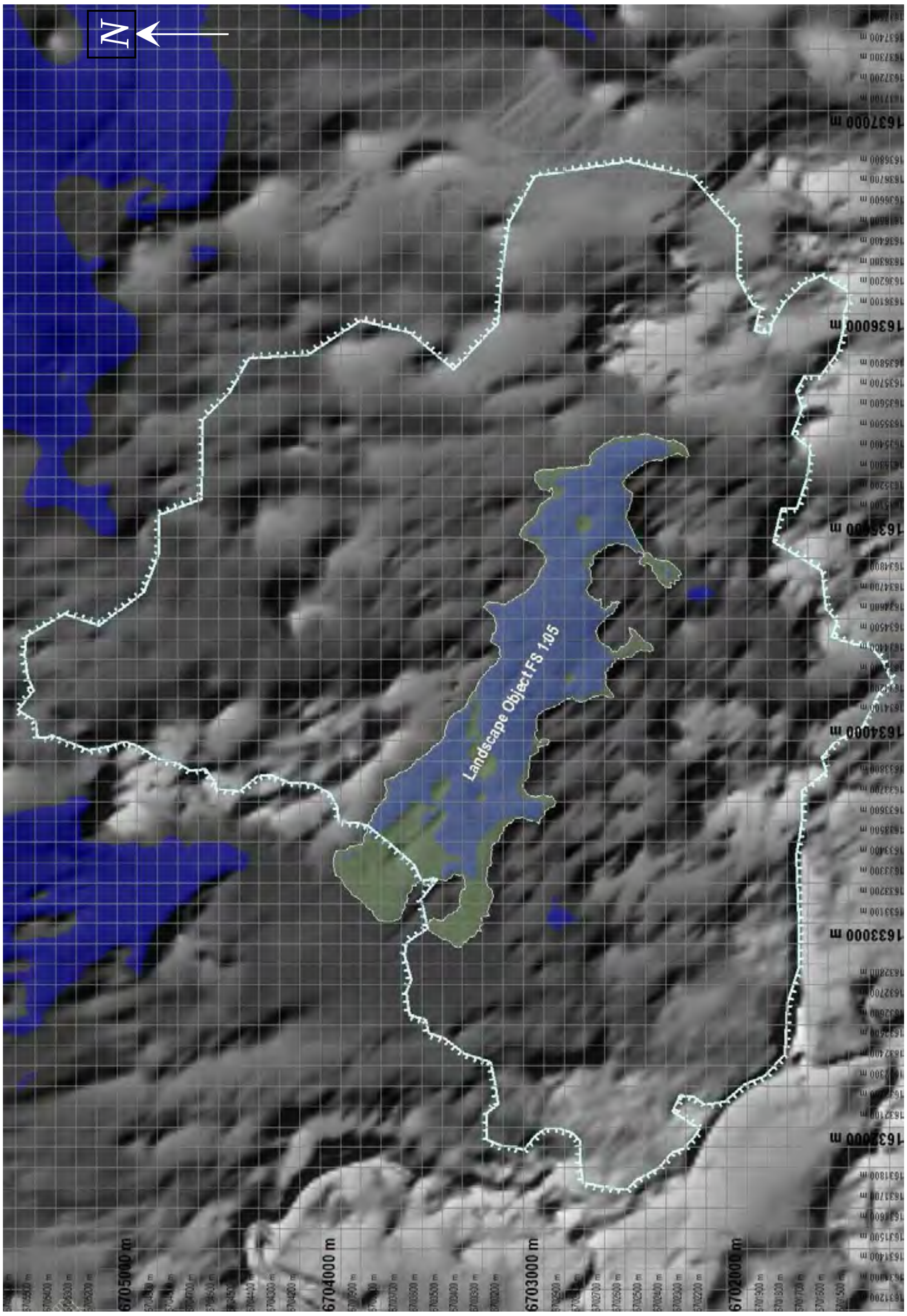

Figure 4-1. A stage in the evolution of the landscape to northeast of the candidate area for the Forsmark spent fuel repository around 4500 CE. Isostatic land rise at 6 mm a^{-1} has led to a fall in local sea level of 15 m relative to the present day. Landscape object FS 1:05 (defined by the -14.5 m contour on the present day bathymetry of the Öregrundsgrepen) has become isolated from the bay, forming first a lake, then a wetland as continued sedimentation fills the lake. The deepest part of the lake is around 3 m and it is assumed that this is the level to which sediment accumulation takes place. The predominant rock type in the regolith is glacial clay of around 5 m thickness. Parts of the basin are accumulating fine sand but the isolation of the bay will lead to accumulations of lake bed sediments to a thickness of around 1.25 m of organic material, mainly gyttja. The outer boundary is Basin 11 from SR-Can (SKB, 2006a). The grid is 100 × 100 m^2. Topographic data courtesy of SKB, used with position. Map plotted with Global Mapper (2009).

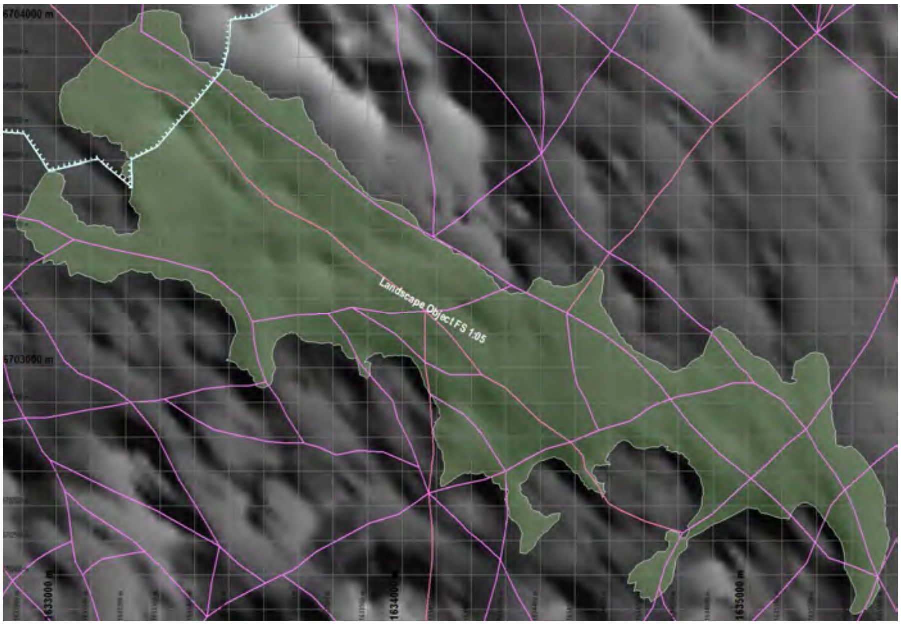

Figure 4-2. The FS 1:05 object in relation to lineaments at the surface. Release to the object is anticipated to be along the fractures into the base of the QD. The grid shows divisions of 10^4 m^2, the default size of landscape elements in GEMA3D. This map shows that there is scope of release to lels in the object over an extended length along lineaments. As groundwater pressure heads change in response to changes in sea level it is possible that the centroid of the release would migrate along the fracture.

Along the centre of the object the mean depth of the organic sediments would then be 1.6 m and it may be anticipated that this would correspond to natural drainage features in the object. Assuming that parts of the wetland area have been converted to agricultural land it may be assumed that artificial drainage has been constructed to drain lakes and wetland areas as well as farmland. Biebighauser (2007) describes a variety of methods both historical and contemporary which would be suitable and effective for similar landscapes. A key feature is that the location of any drainage streams need not coincide with the fractures in the object since drainage pipes would carry excess water towards the human-defined drainage channel. It is therefore justifiable to assume a 100 m width for the agricultural lels.

Typically it might be assumed that artificial drainage is emplaced at a depth of around 1 m (3 to 4 feet according to Biebighauser). The drained water from the surface would then be directed out of the area by a drainage stream carrying all of the run off for the catchment. In studies of land reclamation in the Netherlands (Smedema & Rycroft, 1983) note that, following the initial emplacement of drains, excess water in the surface layers is rapidly lost through evapotranspiration.

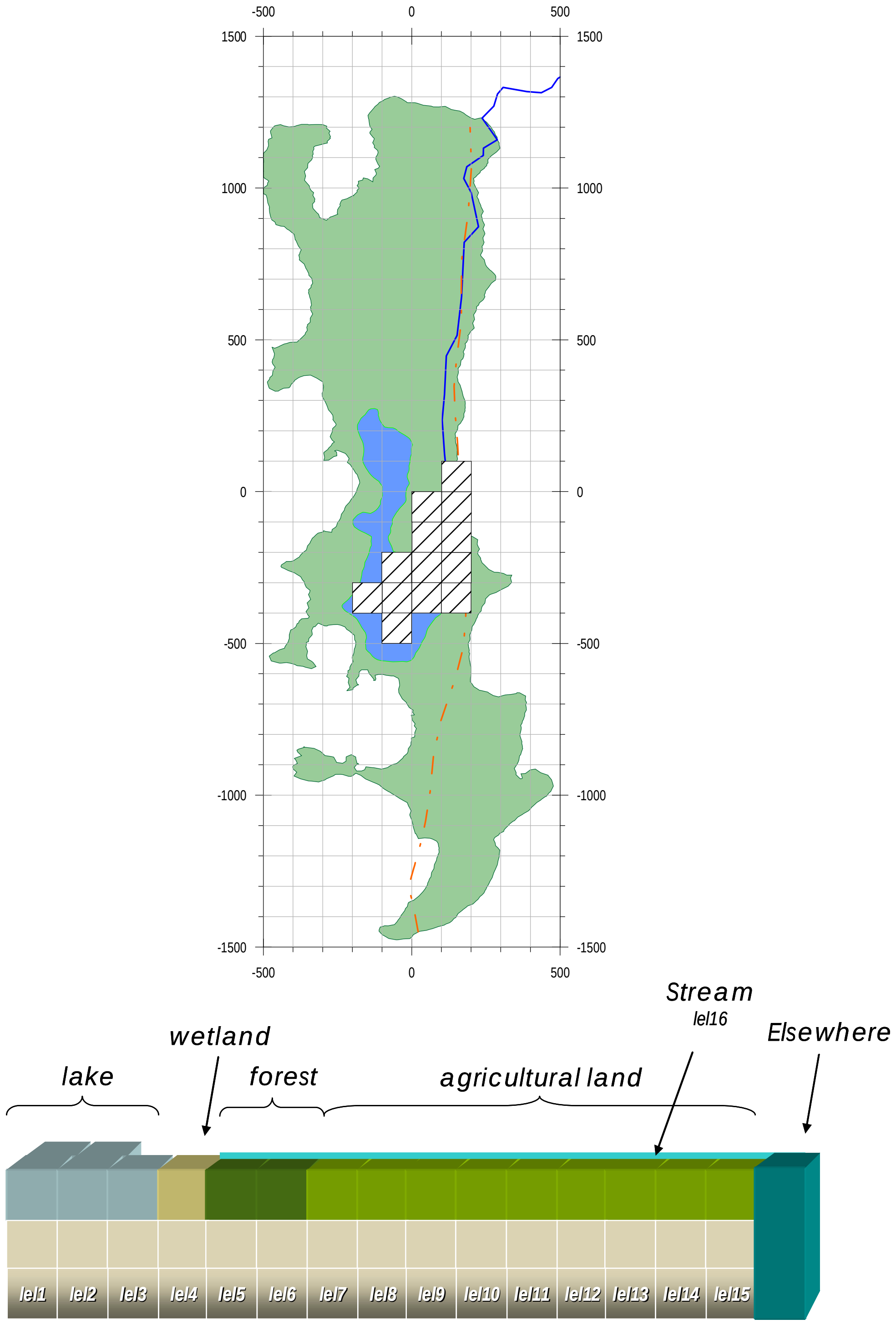

Figure 4-3. Conceptual model of the landscape object for PA purposes. Assuming that a lake, bordered by a wetland, remains at the lowest part of the landscape object a sequence of lels can be determined into which activity released to the base of the QD can migrate and accumulate. The longitudinal extent is 15 lels (each 100 m in length giving a total length of 1.5 km (cf Xu et al. 2008) and has a transverse resolution of one lel. Each of these lels may receive a portion of the overall release. For example purposes each of the ecosystems types lake, wetland, forest, agricultural land and stream, appear at least once in the model.

Thereafter the drainage network begins to function normally[5]. Infiltration and fracture discharge will move through the drained layer to the drainage stream. This provides further justification for modelling the PA lels as wider blocks of QD.

The final conceptualisation of the PA model is shown in Figure 4-3. The model is essentially linear. Diffusion into adjacent compartments is possible but at insignificantly low rates so that it is reasonable to focus on the lels comprising the flow system.

During the bay/lake/wetland phases of development, production is so limited and/or concentrations so low that it is unlikely that any significant doses could arise. The main point of interest is the accumulation of nuclides in the QD of future farmland. Only in agricultural land are the land areas so small that high concentrations combined with cultivation and usage of contaminated material can take place with sufficient intensity to lead to the highest of consequences within the landscape setting.

4.2 System description

From Figure 4-3, the system may be described as follows:

- General description

  There is a fracture aligned with the object through which contaminated water discharges (at ~ 0.06 m a^{-1}). Above the bedrock is around 1.6 to 2 m of QD – the result of the infilling of the object during the principal lake/wetland phase. The result of the infilling is a large area of flat QD material of organic nature (*gyttja*). In limnic and wetland ecosystems the QD is saturated with overlying water in lakes and streams. The upper layers of forests are unsaturated but to a fairly shallow depth (a few tens of centimetres). Agricultural land is assumed to be drained and a network of underground pipes are assumed for this purpose (see Biebighauser, 2007). The upper 1 m of agricultural land is unsaturated and below this level a small local aquifer drains towards a managed stream. The source of radionuclides is the fracture discharging to the base of the QD. Release from the fracture is 1 Bq a^{-1} to each lel.

  There is a lake (300 × 100 m^2) which drains through marginal wetland (100 × 100 m^2) and forest (natural/semi-natural – 200 × 100 m^2) areas. A stream provides drainage from the wetland and the agricultural fields adjacent to the lake. The length of the agricultural land is 9 × 100 m and each agricultural element is 100 m wide. The stream is 900 m long and has a width of 1 to 2 m depending on requirements).

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5 This may be of interest for ^{129}I. George Shaw (Oversite/CLIMB) has noted that the k_d of iodine might be expected to rise with increasing oxidation of the surface soils. Any ^{129}I accumulations in the wetland soils would therefore not necessarily be diminished by drainage because the water would be lost by evaporation leaving the ^{129}I in place. With improved drainage the k_d would increase leading to higher retention of ^{129}I in the surface soils during cultivation.

Table 4-1. Compartment classification system based on the SR97/SR-Can database. The database distinguishes between "soil", "organic" material and "fresh water" conditions.

	Lake	Lake	Lake	Wetland	Forest	Forest	Agri	Agri
lel	1	2	3	4	5	6	7	8
t	f. water	f. water	f. water	organic	organic	organic	soil	soil
d	organic	organic	organic	organic	organic	organic	organic	organic
q	organic	organic	organic	organic	organic	organic	organic	organic
	Agri	Agri	Agri	Agri	Agri	Agri	Agri	Stream
lel	9	10	11	12	13	14	15	16
t	soil	soil	soil	soil	soil	soil	soil	f. water
d	organic	organic	organic	organic	organic	organic	organic	f. water
q	organic	organic	organic	organic	organic	organic	organic	organic

Table 4-2. Assumed compartment dimensions in the landscape elements. Overall QD thickness in the model is 2 m. The surface system, in which significant amount of water flow is assumed to be the top 1 m of the QD.

ecosystem	Lel #	l_q [m]	l_d [m]	l_t [m]	surface water [m]	total QD [m]	surface area [m^2]	external catchment [m^2]
lake	1	0.9	0.1	1.0	1.0	1.0	10000	30000
lake	2	0.9	0.1	1.0	1.0	1.0	10000	30000
lake	3	0.9	0.1	1.0	1.0	1.0	10000	30000
wetland	4	0.4	0.1	0.5	0	1.0	10000	0
forest	5	0.5	0.3	0.2	0	1.0	10000	0
forest	6	0.5	0.3	0.2	0	1.0	10000	0
agri	7	0.4	0.3	0.3	0	1.0	10000	0
agri	8	0.4	0.3	0.3	0	1.0	10000	0
agri	9	0.4	0.3	0.3	0	1.0	10000	0
agri	10	0.4	0.3	0.3	0	1.0	10000	0
agri	11	0.4	0.3	0.3	0	1.0	10000	0
agri	12	0.4	0.3	0.3	0	1.0	10000	0
agri	13	0.4	0.3	0.3	0	1.0	10000	0
agri	14	0.4	0.3	0.3	0	1.0	10000	0
agri	15	0.4	0.3	0.3	0	1.0	10000	0
stream	16	0.9	0.1	0.5	0.5	1.0	1800	0

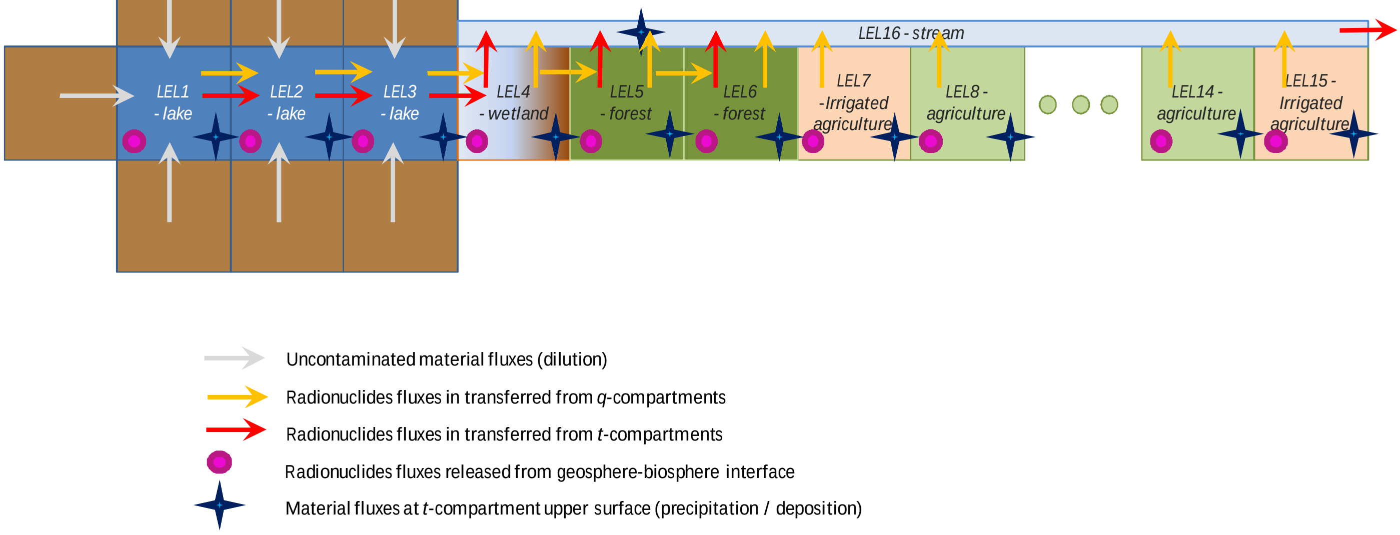

Figure 4-4. Schematic representation of the local hydrology for the lels in the landscape. In this example system Each of the lake lels has adjacent uncontaminated parts of the lake. This causes inflow from the water compartment (t-layer) and from the underlying aquifer (q-compartment). Release to each of the lels is from the fracture beneath the q-compartment. Surface layer drainage coexists with aquifer drainage in the lake/wetland/stream system. There is also runoff form the forest to the stream. Drainage in the agricultural land is via buried drains and this is assumed to flow directly to the aquifer under the stream where it discharges to the stream bed. Representative water fluxes in the model are illustrated in Appendix D.

Data are taken from the SR97 dataset used by SKB in SR-Can assessment. Though the k_d database, in particular, is not the most representative of typical conditions, the old dataset allows comparison with the results of the earlier GEMA modelling which used the same database. K_d values for organic soils and sediment are used except for the water compartments (lakes and streams and the top layer of agricultural lels, see Table 4-1). Grain density of soils and sediment is taken to be 2650 m^3 kg^{-1}. The compartment dimensions in the sixteen lels are shown in Table 4-2 for the different ecosystem, types. The full dataset is reproduced in Appendix C.

- Water table, landscape hydrology and exfiltration to the lels

No external catchment is included although the model structure allows it. There is input to the bottom of the lel (groundwater input from the fracture but no external uncontaminated water) as well as input at the top from precipitation (but no runoff from the catchment). The excess of accumulated water in the lel moves downstream from the q-compartment to the stream lel. For the lake area it is reasonable to allow uncontaminated flows from the larger lake to dilute the flux in the release lel before flow downstream. The hydrology is illustrated in Figure 4-4.

Below the 1 m level the QD is saturated and consists of clays in which the water movement is slow because of low hydraulic gradients and low permeability. The q-level of the model is permeable and acts to drain the system. Below the stream it is permanently saturated. This compartment forms the aquifer from which well abstraction may take place.

The saturated level is in the geosphere-biosphere interface (ie, the deeper QD, below 1 m) This is maintained by drainage in the q-layer to the stream.

The exact location of the fracture in relation to the stream is not known. The stream is placed by humans for their convenience and is maintained to provide drainage for the flat area at the bottom of the catchment. **It need not necessarily coincide with the stream** though it may do in reality. **It is therefore assumed that release is to the q-compartments of the lels**. There is no direct release to the stream lel since this would rapidly lead to nuclides being lost downstream. As with the lack of catchment dilution, this is a conservative modelling assumption.

- The lake (lels 1 – 3)

There has been reluctance in the past to accept SKB's assertion that there is no water flux through the deeper QD at the bottom of lakes and wetlands, with their assumed release passing from the bedrock directly to the water compartment. However, the discussion in Smedema & Rycroft (1983) supports this view. Because the fracture extends along the lake there might be a situation where seepage would enter lake water through peripheral sediments (the d-compartment in GEMA3D). The discharge would still pass through and interact with the sediments and the situation of a direct release from the bedrock to the water column is again ruled out. Anders Wörman (private communication) suggests that discharge to the whole of the sediment compartment in the lel is reasonable and so the small 0.06 m a^{-1} flux from the fracture (cf. SR-Can, SKB, 2006a) is assumed to pass through the main bulk of the QD. The volumetric flow from the fracture must use the area of the fracture – typically 1.5 km long by the width of the fracture, 2×10^{-4} m (Broed & Xu, 2008), giving a water flux over the whole fracture of 6×10^{-3} m^3 a^{-1}. This is a much smaller volumetric flow the meteoric input. It's primary importance in the model is to drive the radionuclide release. Sensitivity analysis shows that the results are not influenced by this parameter. Nevertheless a better description of the hydrology of the geosphere-biosphere interface in future modelling is to be preferred

Water in the lake is clearly **not** from deep discharge. There is precipitation: the total area of the lake is, say 9 lels = 9×10^4 m^2. The input directly from the atmosphere is therefore $d_{ppt} - d_{ETP}$ = 0.6 – 0.4 = 0.2 m a^{-1}. The overall water flux through the lake is therefore 2×10^4 m^3 a^{-1}. This is interpreted to the effect that lel1 receives the output from two uncontaminated lels, lel2, two and lel3, three. For future reference it might be possible to use a single larger compartment for the "uncontaminated" part of the lake in the model.

Sedimentation may also be accounted for in the mass balance scheme (m_{dep}) until the lake is full. A timescale for this process is required and for present purposes the sedimentation parameter in the lake is set to zero[6].

The q- and d- compartments have a porosity 0.3 and are assumed to be saturated.

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6 A major role for the Forsmark surface systems SDM 2.3 (Lindborg, 2008) will be to provide details of solid material transport, as a consequence of the carbon flux models.

- The wetland (lel 4)

  The wetland is one lel in size. In addition to the water flux from the fracture there is net precipitation at the surface. The deepest compartment of the wetland model (q) remains saturated with little water movement, as does the deep compartment (d). Water flows are principally in the t-compartment, only the small flow from the fracture through the q- and d- layers is included. In the t-compartment the net precipitation mixes with the fracture's input and the inflow from the lake.

  In the wetland all compartments are saturated. The q- and d- compartments have a porosity of 0.3 but the t-compartment's value is 0.5. There is small suspended load in q- and d- (10^{-3} kg m^{-3}) but in the t-compartment the value is 0.1 kg m^{-3}. Organic conditions are assumed for all three compartments.

- The forest (lels 5 - 6)

  Two lels are assumed for the forested area. The output of the wetland flows into the first (lel5), through to the second (lel6). Additional water fluxes come from the net infiltration and the fracture. Water is not assumed to flow laterally in the q-compartment but does in the d- and t-compartments.

  Water leaving the forested area is assumed to discharge to the drainage stream, into which all agricultural areas also drain.

  Details of the forest model are limited in the SR-Can database. It is assumed to be a "natural system" and so "organic" is assumed for each compartment in each of the forest lels.

- Agricultural area (lels 7 – 15)

  The nine lels downstream from the forest have each "organic" q- and d- compartments, an assumption neglecting the redox conditions (presumed reducing in q- but oxic in d-). The t-compartment represents the rooting zone of soils and takes the "soils" classification from SR97/SR-Can.

  Only net infiltration and the groundwater discharge enter the lels adjacent to the stream. Water flows through the top soil into the deep soil and the QD, discharging to the stream.

  Irrigation is assumed in lels 7 and 15, but not the others. The main intention of this is to illustrate the effects of irrigation as a means of contaminant transport and accumulation in the top soil in the model. An irrigation demand of 0.5 m a^{-1} is assumed. The source of the irrigation water is taken to be a well in sunk into the q-compartment (see Appendix D).

  The top soil zone is 0.3 m deep and the deep soil zone 0.7 m. The QD is 1 m. There is a bioturbative flux circulating material between the deep and top soil compartments of all agricultural land.

- The stream (lel 16)

  The stream takes the outflow from all lels in the model. It is assumed to be 1100 m long. It has a depth of 0.5 m and width of 2 m. A bed sediment layer of thickness 0.1 m lies above the QD (thickness 1 m).

4.3 Release and geosphere-biosphere interface

The model described here is designed to illustrated the features and potential of the GEMA3D modelling approach. It is not yet a definitive interpretation of the Forsmark system. This will only be possible after a thorough reinterpretation of the Forsmark surface system site descriptive model (SDM 2.3, Lindborg, 2008). An initial review of the final surface system SDM suggests that details of the hydrology (Kłos, 2010) associated with landscape objects on the scale envisaged here, may not be well described. Of particular concern is the lack of detail concerning the release from the bedrock to the base of the QD. For present purposes release is assumed to be from the "geosphere" into the base of the "biosphere" model as represented by the q-compartment.

4.4 Illustrative results

4.4.1 Concentrations

To illustrate the workings of GEMA3D releases of ^{129}I and ^{226}Ra are employed (^{210}Pb and ^{210}Po growing in). GEMA3D calculates inventories and corresponding concentrations. Results for the concentrations are used here. They are calculated as follows:

- Volumetric concentrations in q-, d, and t-

$$C_i = \frac{N_i}{V_i} \text{ Bq m}^{-3},\ i = q, d, t. \tag{4.1}$$

- Porewater concentrations in q- (aquifer / well water concentration)

$$C_{pq} = \frac{1+\alpha_q K_q}{\theta_q + (1-\varepsilon_q)\rho_q K_q} \frac{N_q}{V_q} \text{ Bq m}^{-3}, \tag{4.2}$$

Results for concentrations in top soil (surface water where present) and porewater in each of the compartments are shown in Figure 4-5 and Figure 4-6, respectively.

The effect of radionuclide k_d are clearly seen, particularly for the top soil. The assumed hydrology in this example suggests high concentration in the aquifer beneath the "forest" are possible. This is because the entire outflow from the lake passes first through the wetland t-compartment before entering the forest q-compartment. This is probably less than accurate: the wetland should drain directly to the stream.

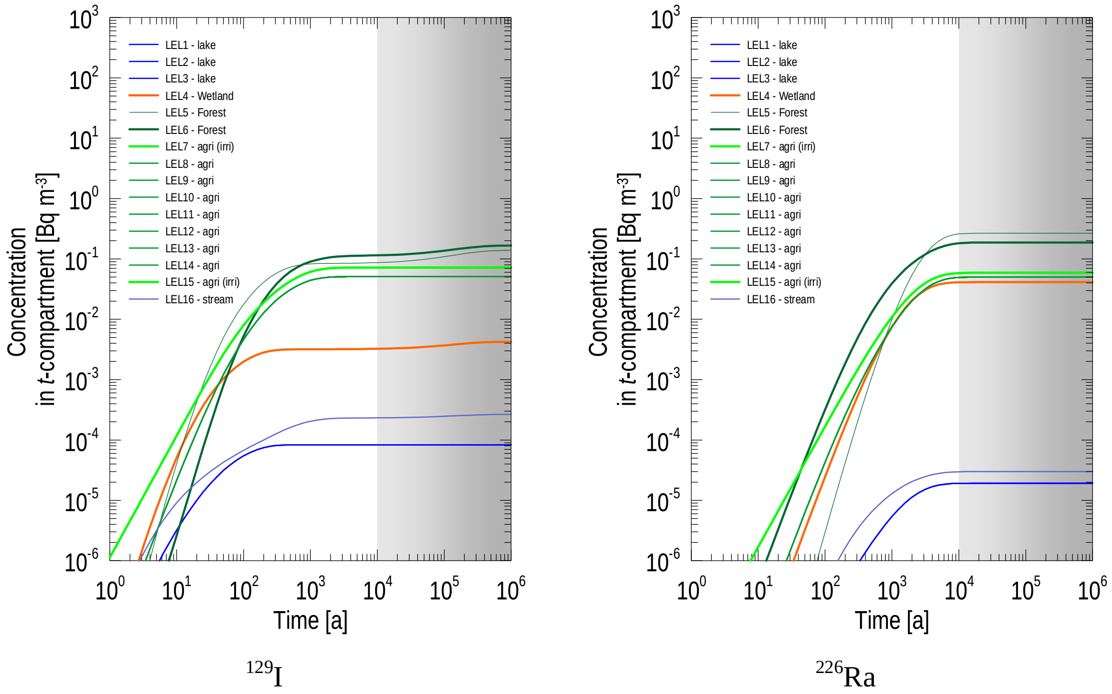

Figure 4-5. Concentration of ^{129}I and ^{226}Ra in the t-compartment.

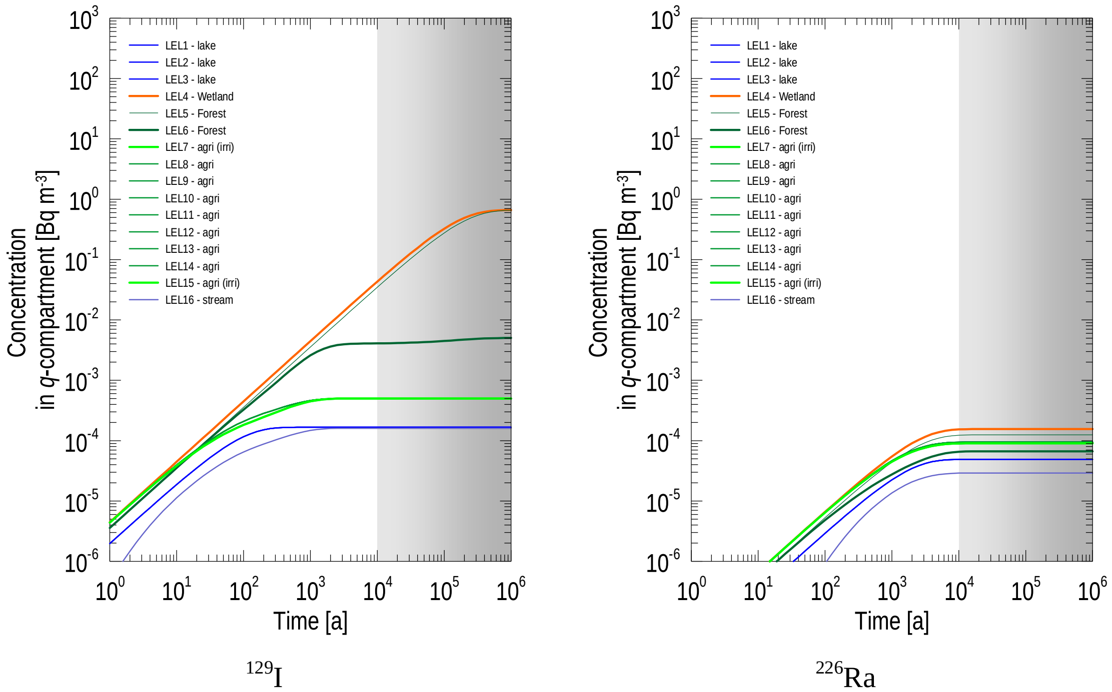

Figure 4-6. Concentration of ^{129}I and ^{226}Ra in the porewater of the q-compartment

The plots are colour coded according to ecosystem type. Broadly each ecosystem type gives similar results. This is a consequence of the way in which the hydrology is interpreted here. In retrospect is was not necessary to model each of the non-irrigated agricultural areas, and only a single irrigated area is of radiological concern. However, this may change with a better interpretation of local conditions. These results suggest, however, that with limited information, it is reasonable to model individual lels independently. Only in the case where there is flow of water from one forest lel to the next is it possible to distinguish results from each forest model.

4.4.2 Doses

In the generic system there are a number of doses that can be calculated. Depending on the type of ecosystem and societal context these can be combined in a number of different ways to give the radiological impact of the release. Accumulations in the lel which might subsequently become available for dose can be used on this basis to calculate *latent doses* (see Section 4.5).

There are four types of dose calculated: inhalation doses (from suspended particulates), external irradiation (from groundshine), drinking water and foodstuff ingestion. The inhalation dose,

$$D_i^{inh} = H_{inh} O_f a_{dust} I_{inh} \frac{C_i}{(1-\varepsilon_i)\rho_i + \theta_i \rho_W} \text{ (Sv a}^{-1}\text{)}, \tag{4.3}$$

uses the dose per unit intake on inhalation (H_{inh}, Sv Bq^{-1}), the fractional annual occupancy factor for the lel (O_f, -), the airborne dust load (a_{dust}, kg m^{-3}) and the annual inhalation rate (I_{inh}, m^3 a^{-1}), together with the dry weight concentration in the source compartment.

External dose is

$$D_i^{ext} = O_f G \frac{C_i}{(1-\varepsilon_i)\rho_i} \text{ (Sv a}^{-1}\text{)}, \tag{4.4}$$

Using the wet weight concentration, occupancy factor and the nuclide's external irradiation conversion factor (G (Sv a^{-1})(Bq m^{-3})$^{-1}$)

Drinking water doses are simply calculated from the concentration in the source of the water:

$$D_i^{dw} = H_{ing} I_{dw} C_i \text{ (Sv a}^{-1}\text{)}, \tag{4.5}$$

where H_{ing} (Sv Bq^{-1}) is the dose per unit intake on ingestion.

Ingestion doses area calculated using the aggregated transfer factors introduced by SKB for AR-Can (Avila, 2006). This approach gives the dose from food ingestion related to the concentration in the QD, top soil or water compartment. For each of the compartments, then, different foodstuff ingestion doses can be calculated for different ecosystem types, with different combinations of foodstuffs included in the derivation of the aggregated transfer factor (TFagg) value. In these calculations the TFaggs provided for SR-Can by Avila are used and the following doses are calculated:

$$\begin{aligned}
D_i^{nat} &= f_c^{nat} H_{ing} I_C TF_{agg}^{nat} \frac{C_i}{(1-\varepsilon_i)\rho_i} \\
D_i^{agri} &= f_c^{agri}{}_c H_{ing} I_C TF_{agg}^{agri} \frac{C_i}{(1-\varepsilon_i)\rho_i} \quad (\text{Sv a}^{-1}). \\
D_i^{fw} &= f_c^{fw} H_{ing} I_C TF_{agg}^{fw} C_i \\
D_i^{irri} &= f_c^{irri} H_{ing} I_C TF_{agg}^{irri} C_i
\end{aligned} \tag{4.6}$$

The TFaggs are given for four types of ecosystem. Two of these relate the dose to the *soil compartment* from which primary production is generated: natural ecosystems (wetlands and forests), agricultural land. The remaining two are based on water concentrations (lake or stream) for freshwater ecosystems[7] and irrigation source for irrigated ecosystems (stream, lake or local aquifer). The carbon intake requirement of an adult is I_C (kgC a^{-1}). To account for the area of the lel required to produce the required carbon intake, there is an ecosystem specifc areal correction factor which takes account of the details in Table 2-1:

$$f_c^{eco} = \begin{cases} 1 & A \geq A_{10}^{eco} \\ A \big/ A_{10}^{eco} & A < A_{10}^{eco} \end{cases} \quad (\text{-}). \tag{4.7}$$

where *A* is the area of the lel and A_{10}^{eco} is the area required to produce sufficient carbon for ten adults.

Radiological impact of the accumulations is evaluated by combining doses from a range of sources. The generic total dose from a lel is given by

$$D_{tot} = D_{inh} + D_{ext} + D_{dw} + D_{food}^{eco} \quad (\text{Sv a}^{-1}), \tag{4.8}$$

however, taking account of the ecosystem types, and the compartments involved the dose pathways and the total dose are evaluated as shown in Table 2-1. Total dose for selected lels are shown in Figure 4-7.

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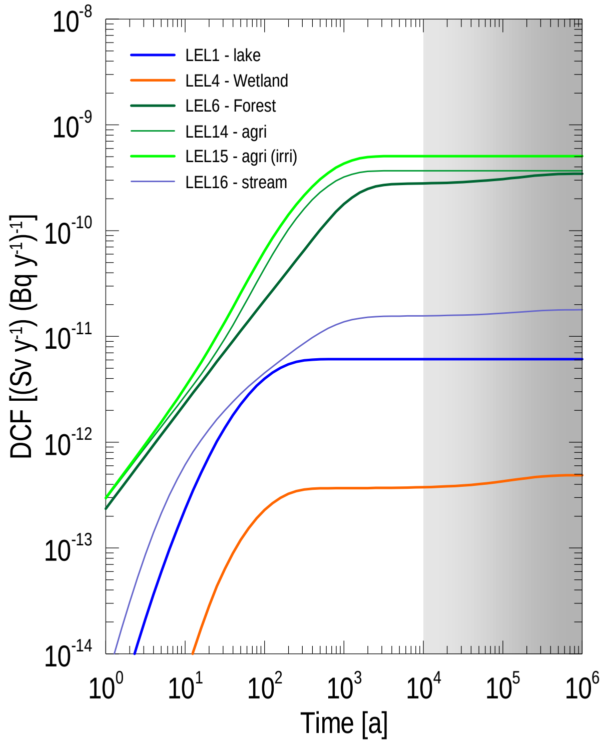
[7] NB, we do not consider marine ecosystems here, thought here is no reason why the same format could not be adopted.

Table 4-3. Compartments involved in calculation of dose for each lel in the model. Non-shaded entries are used in the calculation of total dose. Shaded entries are used to calculate latent doses.

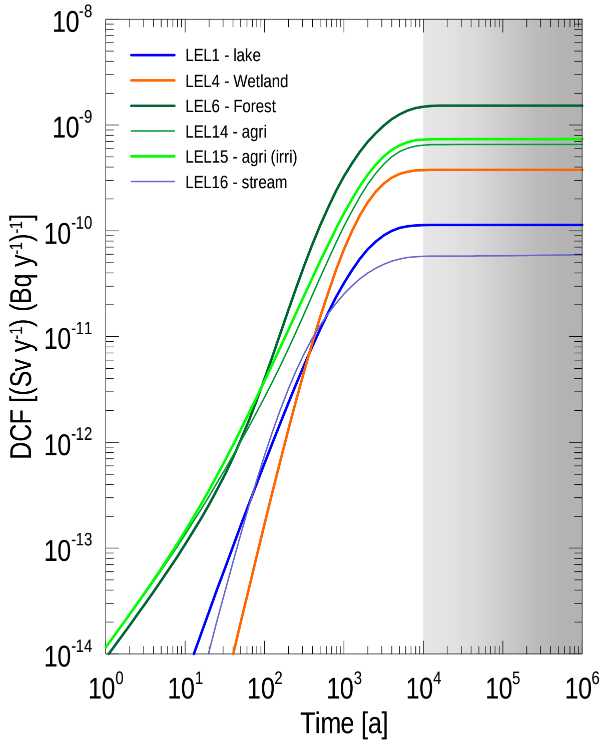
					Ecosystem foodstuff dose			
Lel	Ecosystem type	inh	ext	dw	Nat	Irri*	Agri*	FW
1	lake	C_q	C_q	C_t	C_q	C_{pq}	C_q	C_t
2	lake	C_q	C_q	C_t	C_q	C_{pq}	C_q	C_t
3	lake	C_q	C_q	C_t	C_q	C_{pq}	C_q	C_t
4	wetland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_q	-
5	forest	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
6	forest	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
7	irrigated farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
8	farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
9	farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
10	farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
11	farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
12	farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
13	farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
14	farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
15	irrigated farmland	C_t	C_t	C_{pq}	C_t	C_{pq}	C_t	-
16	stream	C_q	C_q	C_t	C_q	C_{pq}	C_q	C_t

* Avila (2006) calculates TFaggs for both agricultural land and irrigated land. The difference is that the irrigation TFagg is used with the concentration in the aquifer water in this case (or stream or lake water, as required). Agricultural land is used with the topsoil concentration calculated from the t-compartment of the lel. For lels 7 and 15 in this model there is irrigation using aquifer water (the q-compartment) and this contributes to the concentration in the t-compartment. In conjunction with the TFagg for agricultural land, this gives a higher dose than that from the irrigation TFagg in combination with the porewater concentration in the q-compartment of the irrigated lels. For this reason the agricultural dose is used in the calculation of the total dose from the irrigated lels.

Figure 4-7. Total dose from selected lels in the landscape model.



(a) ^{129}I



(b) ^{226}Ra chain

Each lel receives 1 Bq a^{-1} so the Dose conversion factor for each lel is numerically equivalent to the calculated dose. For ^{129}I and the ^{226}Ra chain the maximum DCFs are around 10^{-9} Sv Bq^{-1}, broadly inline with recent simulations (eg, Kłos, 2008a, 2009). These values take account of the area required. For a single (albeit, somewhat unfortunate) individual the maximum DCF could be a factor of ten higher.

The dynamics shown in the two plots reflect the different sorption characteristics of ^{129}I and ^{226}Ra and its daughters. Equilibrium is established for the weakly sorbing ^{129}I after around one thousand years, as concentrations in the top soil stabilise. There is an increase in the wetland and forest doses due to the rapid equilibration of the top soil concentration over 100 to 1000 years (associated with release to adjacent compartments with inflow to the t-compartment) but the accumulation in the q-compartment takes longer as there is little diluting flow in the QD of the lake, wetland and forest. Because the agricultural lands are drained the concentration in the aquifer porewater never rises as high as it does in the undrained lels.

The more highly sorbing nuclides of the ^{226}Ra chain are retained in the q-compartment of the model, even when the lels are well drained (Figure 4-6). The porewater concentrations are therefore lower but, when they reach the t-compartment, the nuclides are retained there. This is important because it influences the exposure pathways influencing total dose. Figure 4-8 shows the calculated exposure pathways for each of lel4 (wetland), lel6 (second forest lel) and lel15 (irrigated agricultural land). For ^{129}I the natural foodstuff consumption dominates the wetland dose (notwithstanding the small areal correction factor of 2.73×10^{-3}) whereas for the ^{226}Ra chain the total dose is dominated by the inhalation dose from accumulations of ^{210}Po in of the wetland.

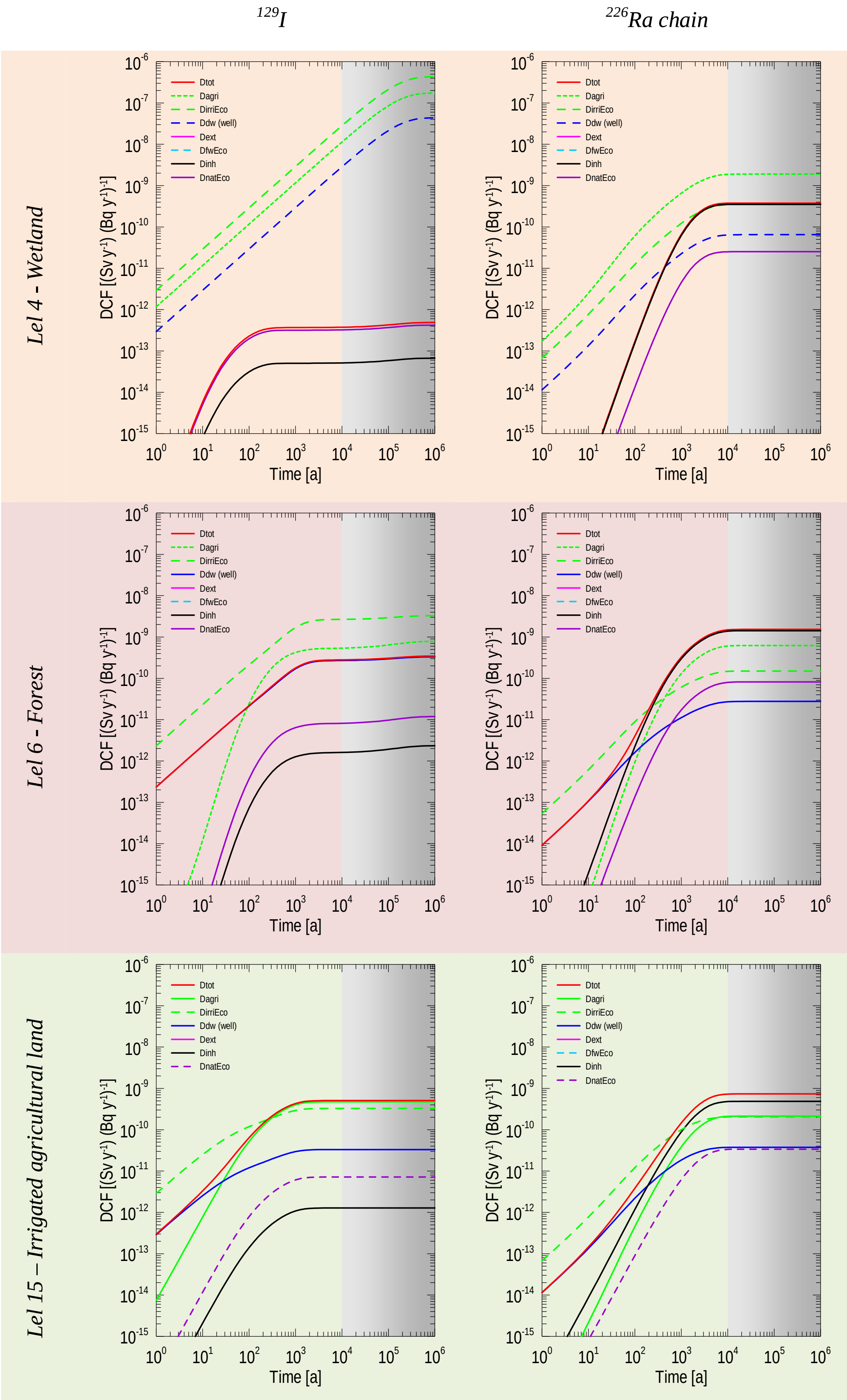
In the second of the forest lels (lel6) a well is assumed to be possible in the QD, this is done for illustrative purposes with the result that the drinking water dose from well water dominates the total dose for ^{129}I. As with the wetland it is the accumulation of ^{210}Po in the t-compartment that dominates the total dose from the ^{226}Ra chain, again via the inhalation dose.

In the agricultural land of lel15, the irrigation of the topsoil leads to higher concentrations of both ^{129}I and the ^{226}Ra chain in the t-compartment. Agricultural foodstuff consumption dominates for ^{129}I. For the chain, the inhalation dose is again the most important contribution to total dose but the foodstuff dose is similar. Also shown in Figure 4-8 are the latent doses (dashed line). In the irrigated agricultural lel the higher foodstuff dose from accumulations in the irrigated top soil is seen to be somewhat higher than the corresponding dose calculated on the basis of the concentration in the aquifer porewater alone. For this reason the top soil concentration is used in the estimation of total dose.

4.5 Latent doses and step change

The latent doses also calculated in this model illustrate the potential for future exposures on system change. The most striking illustration in Figure 4-8 is that of ^{129}I in the wetland. Because high local concentrations can build up in the q-compartment there can be high doses *if this material is converted to alternative use.* As a wetland agricultural/irrigated foodstuffs do not arise. However, the indication is that the interpreted hydrology of the lel could give rise to significant doses at later times were the wetland to be converted to agricultural usage. Similar comments apply to the ^{226}Ra chain results.

Figure 4-8. Dose conversion factors by pathway in selected lels. Solid lines are those pathways used to calculated the total dose in each lel. Dashed lines are latent doses.



It may be noted that the latent doses from agricultural systems do not exceed the evaluated total dose. This is because agricultural doses take account of more pathways than the other ecosystem types, reinforcing agricultural systems as the main system of interest in long-timescale dose assessments. In the forest system, the accumulations of the chain daughters also outweigh the latent dose contribution.

Obviously doses from the latent pathways will not arise in this way. The issue is the potential for the long term accumulations to become available for dose. Of particular interest is the issue of the conversion of wetland to agricultural land. Dose transients have been noted as potentially radiologically significant (Kłos, 2008b). Here the focus is on a potentially more restrictive system in which there is very little local dilution in the QD above the fracture, leading to high accumulations of nuclides in the QD beneath wetlands.

A simple way to investigate this is to use the concentration after 10, 100, 1000 ka in wetland as the starting point for agricultural land concentrations, assuming that the total inventory in the three compartments of the lel are well mixed at the end of these time periods. The initial inventories are then as shown in Table 4-4. For ^{129}I there are significant differences between the inventories at the three times. For the members of the chain the differences are of less significance. Results are shown for total dose in Figure 4-9.

As expected, this initial inventory scenario has the greatest effect for ^{129}I. For the members of the ^{226}Ra chain the inventories at each of the times are similar. Initially, on conversion to agricultural land there is a relatively high content of the chain members in the upper soil though these leach away gradually. Higher doses arise initially, though they decay to the long-term equilibrium levels over a period of around 1 to 10 ka. Irrigation has the effect of removing radionuclides from the top soil slightly faster than in the case of the non-irrigated land. The initial DCF from converted wetland would be around 3×10^{-8} Sv Bq-1.

Results for ^{129}I show a similar pattern to that of the ^{226}Ra chain, though the range of results is strongly dependent on the time over which the release accumulates in the QD. The DCF can be one or two orders of magnitude higher (from ~ 10^{-9} Sv Bq^{-1} to ~ 10^{-7} Sv Bq^{-1}) in the case where there is long term accumulation in the QD beneath a wetland with subsequent conversion to agricultural land. In this case the availability of ^{129}I in the aquifer means that the irrigated value is slightly higher than the case for non-irrigated land, though the effect is small. Of more interest is the *increase* in dose relative to the initial conditions. This appears to be a result of the high throughflow of water from the shallow aquifer through the deep soil layer into the topsoil as a results of evapotranspiration.

In these models a chronic release to the bas e of the q-compartment is maintained in addition to the initial condition release. The calculated doses return to their long term values seen in the earlier scenarios after around 5 ka.

Table 4-4. Initial inventories in the thee lel compartments at 10, 100 and 1000 ka. The "calculated" values are taken from the wetland lel inventories at the times indicated. The "well-mixed" inventories use the total "calculated" inventories distributed evenly through the three compartments (implicitly by deep ploughing) prior to use as agricultural land. The initial inventories are therefore calculated according to the depth of the compartments. Both irrigated and non-irrigated agricultural land are investigated.

		"calculated"				"well-mixed"			
time [ka]	compartment	^{129}I	^{226}Ra	^{210}Pb	^{210}Po	^{129}I	^{226}Ra	^{210}Pb	^{210}Po
10	q	9.67E+03	2.28E+03	2.28E+03	2.28E+03	3.88E+03	1.01E+03	1.01E+03	1.01E+03
	d	6.31E+00	3.45E+01	3.45E+01	3.44E+01	2.91E+03	7.55E+02	7.55E+02	7.55E+02
	t	1.62E+01	2.06E+02	2.06E+02	2.05E+02	2.91E+03	7.55E+02	7.55E+02	7.55E+02
100	q	7.28E+04	2.31E+03	2.31E+03	2.31E+03	2.91E+04	1.02E+03	1.02E+03	1.02E+03
	d	1.87E+01	3.48E+01	3.49E+01	3.47E+01	2.18E+04	7.65E+02	7.65E+02	7.64E+02
	t	1.85E+01	2.07E+02	2.07E+02	2.06E+02	2.18E+04	7.65E+02	7.65E+02	7.64E+02
1000	q	1.48E+05	2.31E+03	2.31E+03	2.31E+03	5.92E+04	1.02E+03	1.02E+03	1.02E+03
	d	3.35E+01	3.48E+01	3.49E+01	3.47E+01	4.44E+04	7.65E+02	7.65E+02	7.64E+02
	t	2.11E+01	2.07E+02	2.07E+02	2.06E+02	4.44E+04	7.65E+02	7.65E+02	7.64E+02

Figure 4-9. Dose conversion factors by pathway in selected lels.

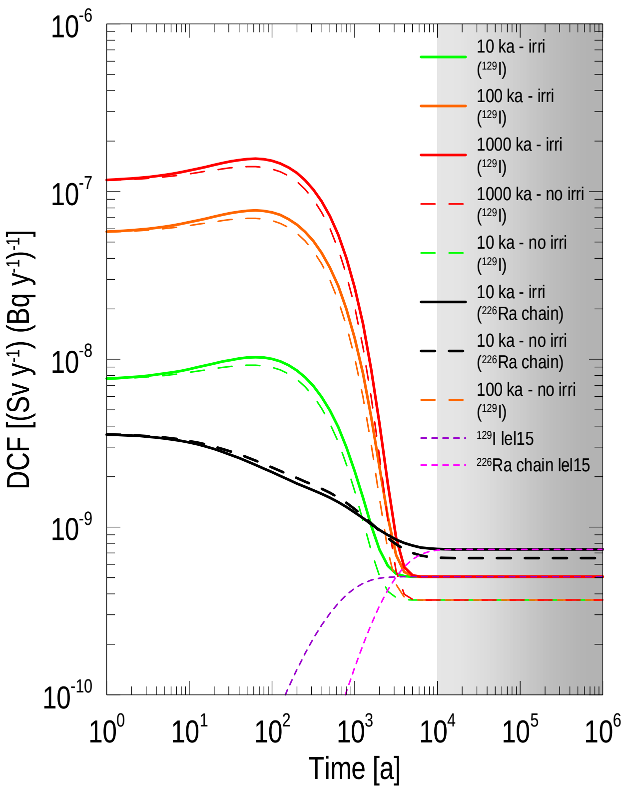


Table 4-5. Solid-liquid distribution coefficients used in this study. Four classification of medium type are used. In the calculations performed here the organic_*classification was used for all media.*

element	class	BE	min	max	notes
iodine	**agri soil**	**3.E-01**	**1.E-01**	**1.E+00**	**Karlsson & Bergström (2002)†**
	freshwater	3.E-01	1.E-01	1.E+00	Karlsson & Bergström (2002)†
	brackish	3.E-01	1.E-01	1.E+00	Karlsson & Bergström (2002)†
	organic	**3.E-02**	**3.E-03**	**3.E-01**	**Karlsson & Bergström (2002)†**
radium	**agri soil**	**5.E-01**	**1.E-02**	**1.E+00**	**Karlsson & Bergström (2002)†**
	freshwater	1.E+01	1.E+00	1.E+02	Karlsson & Bergström (2002)†
	brackish	1.E+01	1.E+00	1.E+02	Karlsson & Bergström (2002)†
	organic	**2.E+00**	**2.E-01**	**2.E+01**	**Karlsson & Bergström (2002)†**
lead	**agri soil**	**1.E-01**	**1.E-02**	**1.E+00**	**Karlsson & Bergström (2002)†**
	freshwater	5.E-02	1.E-02	1.E-01	Karlsson & Bergström (2002)†
	brackish	5.E-02	1.E-02	1.E-01	Karlsson & Bergström (2002)†
	organic	**2.E+01**	**8.E+00**	**6.E+01**	**Karlsson & Bergström (2002)†**
polonium	**agri soil**	**5.E-01**	**5.E-02**	**3.E+00**	**Karlsson & Bergström (2002)†**
	freshwater	1.E+01	1.E+00	1.E+02	Karlsson & Bergström (2002)†
	brackish	2.E+01	1.E-01	5.E+01	Karlsson & Bergström (2002)†, *
	organic	**7.E+00**	**7.E-01**	**7.E+02**	**Karlsson & Bergström (2002)†**

(a) Original SR-Can database

class	element	class	BE	min	max	notes
agri soils (oxic, above water table)	**iodine**	Loam	3.E-02	1.E-03	5.E-01	IAEA (2009)
organic (reducing, below water table)	**iodine**	Organic	4.E-03	4.E-04	6.E-01	Maillant *et al.* (2007)
clay (QD & deep soil)	**radium**	Clay	1.E+00	2.E-01	2.E+00	IAEA (2009)
	lead	Clay	4.E+00	9.E-01	1.E+01	IAEA (2009)
	polonium	Clay	7.E+00	7.E-01	7.E+01	IAEA (2009)
loam, (mature top soil)	**radium**	Loam	1.5E+01	1.2E-02	1.2E+02	IAEA (2009)
	lead	Loam	1.5E+01	3.6E+00	4.3E+01	IAEA (2009)
	polonium	loam	4.6E-01	1.2E-02	1.8E+00	IAEA (2009) †

(b) Alternative k_d database

Notes:

* values in R-02-28 1000 times too big

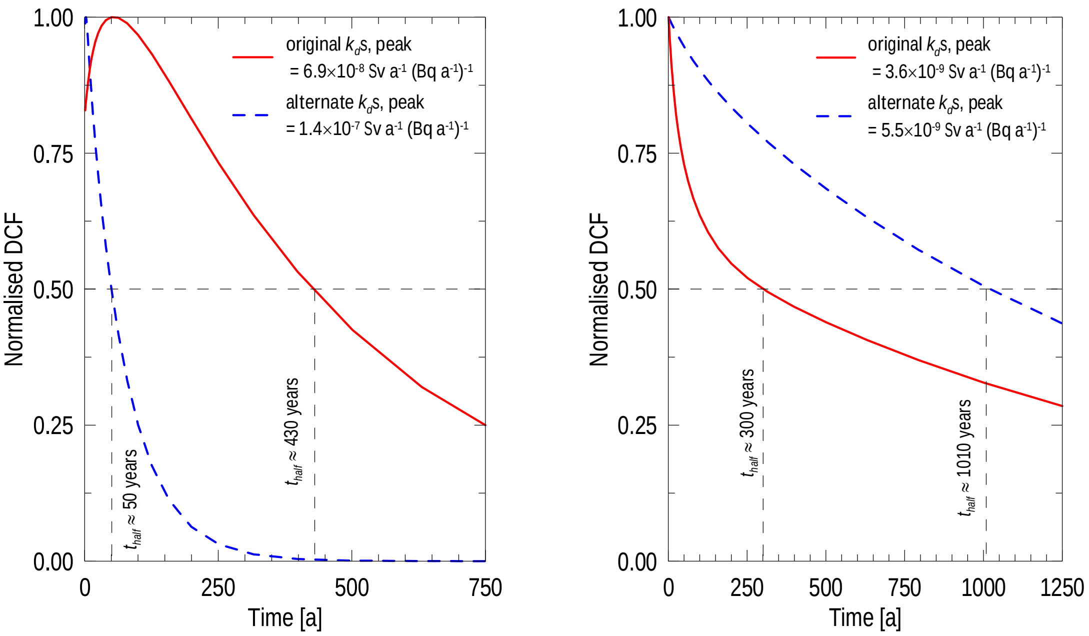
† ranges are BE ± 1 order of magnitude

4.6 Variant k_ds

The previous results are clearly sensitive to distribution coefficient. The reference dataset here is that used in SR-Can and has its origin in earlier work (Karlsson & Bergström, 2002). Since then there have been developments in k_d databases, not least being the recent publication of a site specific k_d database for both Forsmark and Laxemar (Sheppard *et al*., 2009). An alternative k_d database for this study is taken from the recently published IAEA TecDoc 1616 (IAEA, 2009) – providing data for the ^{226}Ra chain in clay and loam, supplemented by Maillant *et al*. (2007) for oxic and anoxic conditions for ^{129}I. The values are shown in Table 4-5. Iodine is a redox sensitive element and a distinction is made between agricultural soils, which are assumed to be well drained and therefore oxic and soils below the water table (the q-compartment) which are assumed to be reducing. An organic classification is assumed for these. The top soil is assumed to be in its "mature" state (cf. Smedema & Rycroft, 1983 and their discussion of reclaimed soils). A "loam" classification is therefore taken for the top soil in the selection of k_d values for top soil. A "clay" classification is selected for deep soils and QD.

Figure 4-10 illustrates results assuming a step change from wetland to agricultural land with the initial inventories in the system determined in Section 4.5. The results are normalised to the peak DCF calculated in each case. Overall, the magnitude of the DCF does not change greatly, as shown in the plots, the revised iodine k_ds are around twice as high whereas for the ^{226}Ra chain, the alternate data result in an increase of around 50%.

Figure 4-10. Dynamics of the initial condition release scenario for irrigated agricultural land derived from contaminated wetland soils showing the influence of alternate k_d datasets. Note the linear scales for these plots.



(a) ^{129}I (b) ^{226}Ra chain

While the effect on the size of the DCF is rather small, the time over which the dose remains near its peak is profoundly altered. The normalisation allows the half time to be illustrated – the time over which the dose remains above 50% of the peak value.

The effect of k_ds is most clearly seen in the case of ^{129}I. With the original dataset, there is a greater retention in the "aquifer" (the q-compartment, below the assumed drainage level). As this is used for irrigation there is a delay to peak dose which arises after around 50 years as a combination of the retention of the initial distribution of activity in the top soil with the accumulation of activity from the irrigation supply. Overall, the dose remains above 50% of the peak for 430 years following the transition. In contrast, the alternate ^{129}I dataset has dose above the peak for only 50 years after the transition and there is rapid leaching of the initial inventory.

The alternate dataset for the ^{226}Ra chain gives a slightly higher DCF, with increased retention in the top soil (~ 1010 years compared to 300 years for the original dataset.

These results demonstrate the sensitivity of the DCF to biosphere k_d. Clearly it is important to get the most appropriate database for the site but it is also important to represent differences in QD chemistry, as typified by the iodine result. Changes in redox through the profile are potentially significant and there is a need to investigate the potential for chemical zonation for redox-sensitive nuclides. An approach to this is presented in Section 5 below.

Even for those elements for which redox sensitivity is not a factor the sensitivity to k_d can be important in this step-change scenario. It has been possible to discount the effects of the dose transient seen on transition from wetland to agricultural land since the spike lasts less that 50 years and Swedish regulations allow for a 50 year integration period (SSI, 1998, 2005) for acute exposures, such as well scenarios (see, Bergström *et al*., 2008). A similar approach applied here might be required, integrating over the highest 50 year period to estimate the DCF.

4.7 A note on local hydrology

As has been clearly stated above, these results are illustrative only and a more detailed interpretation of the SDM database for Forsmark is required in order to model the potential doses for conditions at future Forsmark more reliably. SKB's pre-SR-Can database for the biosphere has been used here. Nevertheless, there are some indications of important features of which we should be aware.

In particular the hydrology of the individual lels in the landscape is important. Local conditions – especially human activities (drainage, land conversion, etc.) are more important than an overview of regional hydrology. The *potentialities* of the site are of concern. The hydrological interpretation of the ecosystems in the lels here is rather simplistic and is not based on a detailed interpretation of likely conditions. However, the interpretation differs somewhat from the earlier SKB view of landscape object hydrology. For comparison the models for the different ecosystems described here are compared with those used by SKB in earlier assessments in Appendix D.

The least well understood part of the system is clearly the geosphere-biosphere interface – the way in which the radionuclide bearing groundwaters emerge from the fractures and mix with the superficial flows of crucial to the evaluation of future radiological consequences. In the q-compartments, which receive the input in this model, a rapid mixing is assumed. The problem of lateral mixing, off-axis relative to the fracture is avoided by assuming a minimum size for lels on a radiological basis, requiring that the area of land is at least large enough to support ten adults under agricultural use. The following Chapter looks at the mobility of radionuclides in the QD above the fracture.

5 TRANSPORT THROUGH THE DEEPER QD

5.1 Quaternary deposits at Forsmark

The GEMA3D biosphere model of the previous chapters describes transport and accumulation in the upper part of the QD. As modelled this has been taken to mean the upper one metre of the QD system. In practice the dose conversion factors (DCFs) employed by SKB are evaluated as the annual individual dose per unit input to the *biosphere*. The release has been assumed to be equivalent to that leaving the fracture. In many cases evaluated in SKB assessments the DCFs are derived from landscape features with high dilution. This is not merely a question of the flux of radionuclides in to the upper part of the QD but also the degree of accumulation and retention.

The QD thickness at Forsmark varies between zero and twenty metres. In those areas likely to be used for agricultural purposes the QD is typically up to six metres thick. The present day agricultural area has a QD thickness of this value. The profile is not homogeneous, however.

Much of the seabed comprises glacial and post-glacial clays of a few metres thickness. Nearer the present day coastline the thicknesses of QD are somewhat lower, possibly as a result of wave action in the littoral zone causing remobilisation of unconsolidated sediment. To the southeast some bays are becoming isolated from the Öregrundsgrepen and considerable thicknesses of sediment are accumulating. In lakes and wetlands highly organic gyttja and clay gyttja is also forming on top of the marine deposits.

As well as the different media comprising the QD the question of the water content – as a surrogate for redox conditions – is also important. As with the upper QD, the issue is essentially the local hydrology. While there is rapid exchange with well aerated meteoric water in the upper QD the question of water flows in the deeper QD remains to be resolved. The model described here looks at the options for representing the deeper QD in a more detailed way. It is not yet a definitive representation of the Forsmark QD but there are useful pointers as to what might be expected from more representative models.

5.2 A simple model for transport in the deeper QD

Xu *et al.* (2008) performed a calculation for a 6 m QD layer assuming a small upward advective flux from a fracture. Advective-dispersive transport was modelled using 60 compartment. This transport takes place in the deeper, saturated and largely stagnant QD below the level of interaction with meteoric waters, with a spatial resolution of 10 cm.

An implementation of the problem has been carried out here based initially on constant conditions throughout the QD column. An aim has been to represent the flux of radionuclides out of the deeper QD and into the base of the GEMA3D model. In the modelling in Section 4, the whole of the release is assumed to be to the base of the GEMA3D q-compartment. The

Table 5-1. Parameterisation and data values for the QD column model, reference values and alternate K_D values..

Parameters	Definitions	Units	Values	References
u_{QD}	Darcy velocity in QD	[m a^{-1}]	0.058	Xu *et al.* (2008)
D	Dispersion coefficient	[m^2/y]	0.0065	Xu *et al.* (2008)
L_{QD}	Thickness of each QD layer	[m]	0.5	Assumed in this report
N	Number of cells in Ecolego discretisation block	[-]	50	Assumed in this report ($\Rightarrow \Delta x$ = 1 cm)
T_{QD}	Total thickness of QD	[m]	5.0	$T_{QD} = NL_{QD}$
ρ_{QD}	Density of QD	[kg/m^3]	1667	Derived from Xu *et al.* (2008)
ε_{QD}	Porosity of QD	[-]	0.91	Xu *et al.* (2008)
θ_{QD}	Volumetric moisture content	[-]	0.91	Saturated conditions
K_D *Reference dataset*	^{129}I	[m^3 kg^{-1}]	0.03	As for GEMA3D q-compartment, SR-Can values (SKB, 2006b).
	^{226}Ra		2.0	
	^{210}Pb		20.0	
	^{210}Po		7.0	
K_D *Alternate dataset for top 100 cm*	^{129}I	[m^3 kg^{-1}]	0.03	Alternate data from Table 4-5
	^{226}Ra		15	
	^{210}Pb		15	
	^{210}Po		0.46	
K_D *Alternate dataset for lower 400 cm*	^{129}I	[m^3 kg^{-1}]	0.004	Alternate data from Table 4-5
	^{226}Ra		1.0	
	^{210}Pb		4.0	
	^{210}Po		7.0	

revised K_D dataset discussed above, has also been used to investigate the effects in changes in chemistry along the QD profile and to demonstrate the modelling tools required.

For a sufficiently high spatial discretisation in the column, advective-dispersive transport can be modelled using a compartment model approximation with upwards and downwards transfers:

$$\lambda_{up} = \frac{v_{QD}}{R_{QD} l_{QD}} + \frac{D}{R_{QD} l_{QD}^2} \text{ a}^{-1}, \tag{5.1}$$

$$\lambda_{down} = \frac{D}{R_{QD} l_{QD}^2} \text{ a}^{-1} \text{ (also valid for the loss term at the top of the column).} \tag{5.2}$$

Assuming that the medium is wholly saturated, the retardation factor is given by

$$R = \varepsilon_{QD} + (1 - \varepsilon_{QD}) \rho_{QD} K_D \text{ -.} \tag{5.3}$$

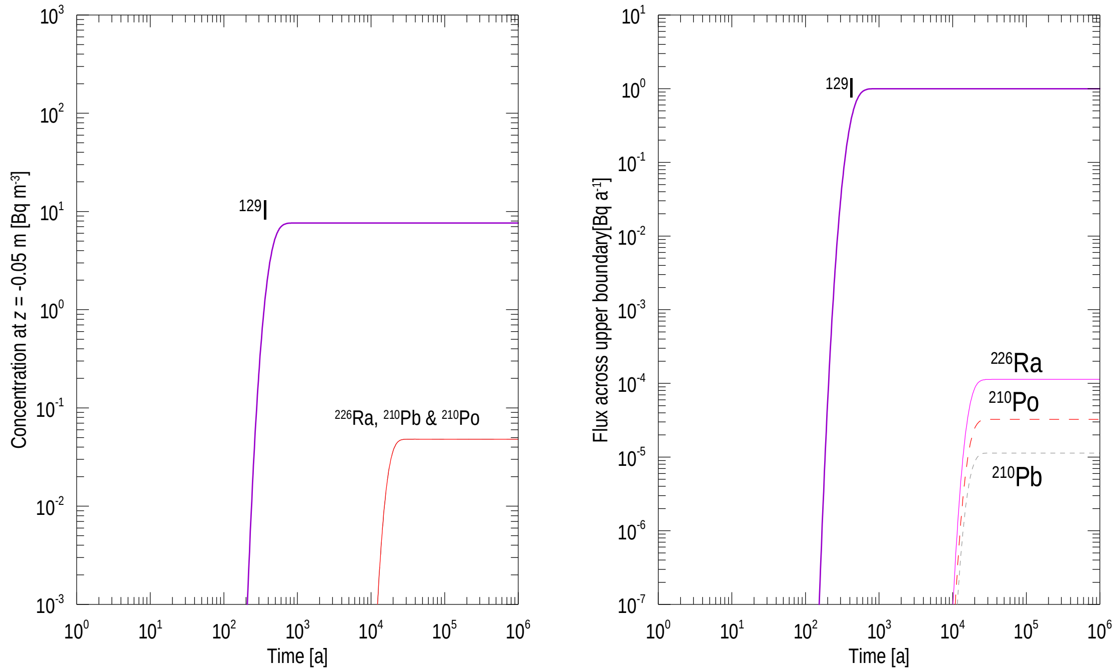
In the implementation of advective dispersive transport here, use has been made of the *Discretisation Block* feature of the Ecolego modelling tool (Broed & Xu, 2008). This allows a column of *N* compartments to be simply constructed using the two transfer coefficients. Within each block, the transfer coefficients given above apply internally between the *N* subdivisions of the block. To simulate different layers in the QD a sequence of 1 m blocks has been used. These transfers also give the rates between the top cell of a lower block and the bottom cell of an upper block. At the base of the column there is no loss, at the top of the column there is a loss term only. This simulates conditions in the QD beneath a water body where there is an implicit rapid turnover above the column (zero concentration boundary conditions).

The higher the value of *N*, the better the accuracy of the numerical approximation. As a test, results from a single 1 m column with 100 cells were compared with those from ten blocks each with 10 cells. There were no differences and it was concluded that the use of multiple discretisation blocks in Ecolego is valid.

The modelling here has prepared the way for multilayer representations of the Forsmark QD if required. Results are presented here for a 5 m thick QD column. There are ten layers based on the values given in Table 5-1. The SR-Can k_d database was used as a *reference case* with the alternative database from Section 4.6 used to investigate the effects of changes in chemical characteristics in the different zones of the QD: different material in the case of the ^{226}Ra chain and zonation caused by different redox conditions for ^{129}I.

Xu *et al.*, quotes SKB (2006b) for the value of the density of the QD material. This is assumed to be the *bulk* density since it is much lower that the 2650 m^3 kg^{-1} assumed for the biosphere material. As bulk density with saturated porosity of 0.91, the grain density of the QD material is the 1667 kg m^{-3} given in the table. This illustrates the potential for variation in the retardation parameters in the QD material. A high organic content might account for the lower grain density of the material compared to the assumed value in the biosphere model. It has also been assumed that the saturation of the layers remains constant at 100% however, in the case of the upper 100 cm of the QD being oxidising it might be expected that the volumetric moisture content would be lower. This would have the effect of increasing the retardation factor but the effect has not yet been incorporated into the modelling.

Figure 5-1. Results for the reference case QD column. 5 m column with a continuous 1 Bq a^{-1} of ^{129}I and ^{226}Ra released to bottom of the column.



(a) Concentration in the upper 1 cm of the column

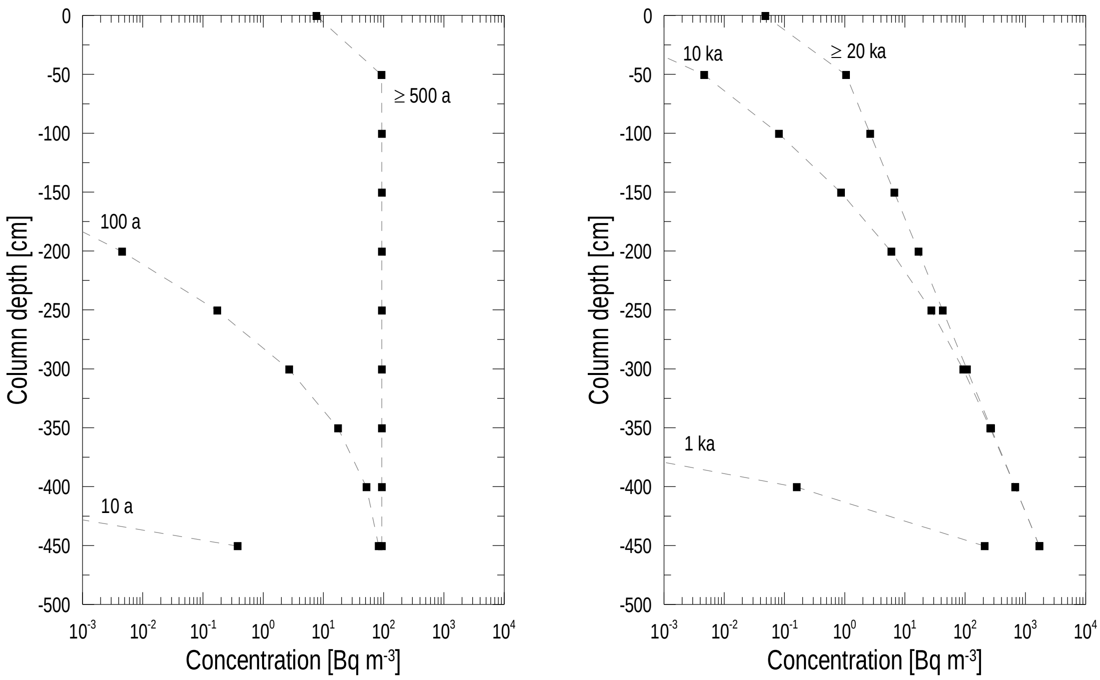
(b) Flux across the upper boundary of the column

5.3 Example results – discussion and analysis

Results are calculated for a 1 Bq a^{-1} input to the base of the column, assumed to be transported with inflowing groundwater with Darcy velocity 0.058 m a^{-1}. Two aspects of the results are shown in Figure 5-1 – the concentration at the top of the column as a function of time and the release flux *across* the upper boundary. For the weakly sorbing ^{129}I the time to equilibrium concentration is around 500 years. The time taken for the flux to equilibrate is similar. For the more strongly sorbed members of the ^{226}Ra chain equilibrium concentrations arise at around 2 ka and the concentration of the three members is equal. The flux takes a similar time to stabilise but there are differences in the flux of the three radionuclides.

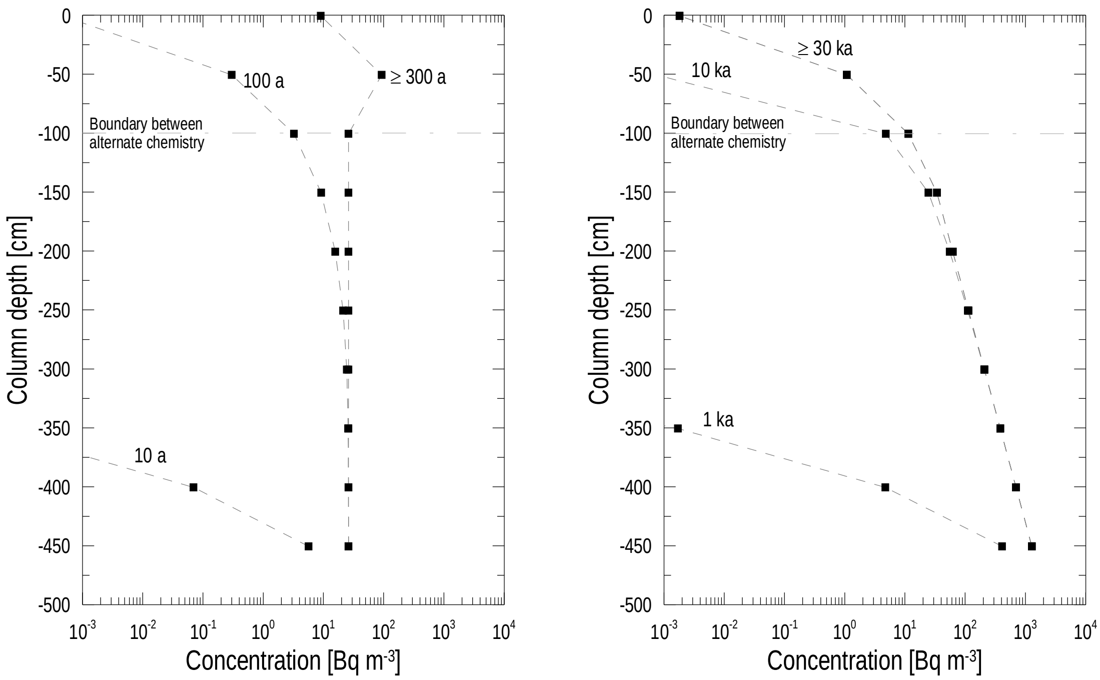
The flux of ^{129}I reaches the input level of 1 Bq a^{-1} but the flux of the chain members is substantially reduced – radium is down by four orders of magnitude but is associated with the input of smaller quantities of the daughters. The release of ^{226}Ra from the *geosphere* (bedrock) is therefore not equivalent to the input of ^{226}Ra to the *biosphere*. Depending on the chemistry and half life of the released nuclide there may be significant effects in the geosphere-biosphere interface – here represented by the 5 m of QD. 1 Bq a^{-1} of ^{226}Ra become 10^{-4} Bq a^{-1} ^{226}Ra plus 3×10^{-5} Bq a^{-1} of ^{210}Po and 10^{-5} Bq a^{-1} of ^{210}Pb into the biosphere, in this reference example. There is therefore scope for dilution in the deeper QD, in terms of the source term to the biosphere. This suggests difficulties of interpretation of the dissociation of geosphere models from biosphere dose models in SKB's assessments.

Figure 5-2. Evolution of ^{129}I and ^{226}Ra concentrations in the 5 m column. For the weakly sorbing ^{129}I equilibrium is reached after around 500 years. For ^{226}Ra the higher k_d requires around 20 ka for equilibrium to be established.



(a) ^{129}I (b) ^{226}Ra

Figure 5-3. Evolution of ^{129}I and ^{226}Ra concentrations in the 5 m column. Results for the alternative K_D dataset. Upper 100 cm have different chemistry to the lower 400 cm.



(a) ^{129}I (b) ^{226}Ra

The main motivation for this study is to investigate models of zonation in the QD. To do this the concentration of radionuclides in the QD column are calculated at the top of each of the ten transport blocks in the model. Figure 5-2 shows the concentration profile as a function of time for the reference dataset. Figure 5-3 gives the same information for the alternate dataset.

The greater mobility of ^{129}I in the deeper QD leads to lower concentrations with a higher concentration in the top 1 m. This illustrates that the effects of chemical zonation based on redox / water content is a practical modelling approach. For ^{226}Ra the lower mobility in the upper part of the modelled profile leads to a lower overall concentration in the top 1 m. The Ecolego transport block offers the possibility of handling zones with varying chemistry in the QD column.

A major influence on the dispersion of activity through the QD block is the groundwater velocity. Equilibrium profiles for u_{QD} = 0.0, 0.0058, 0.58 and 5.8 m a^{-1} are shown in Figure 5-4. Two features are apparent in these results: the higher the Darcy velocity, the lower the overall concentration in the QD column, and the higher the flow the more uniform the distribution.

The first of these features is understood by the assumption of a zero concentration boundary condition at the upper cell of the block, consistent with discharge into rapidly flowing water above the layer. For ^{129}I there is a fairly linear relationship between concentration in the column and the throughflow – the higher the flow the lower the concentration as the weakly sorbing species is washed through the column. The highest concentrations occur for the diffusion only case.

For ^{226}Ra there is the opposite effect. Retardation of ^{226}Ra means that the diffusion only result gives the lowest concentrations. Interestingly, the highest concentration in the profile comes not from the highest water flux, but from the value of 0.058 m a^{-1}. This further illustrates of how a clear understanding of local hydrology is fundamental to the adequate description of the system.

According to SKB the low flow regime is the best description of the hydrology beneath lakes and wetlands at Forsmark. This has been an issue with SKB for a number of years. SKB maintain that there is little likelihood of releases to the bottom of lakes and wetlands because the deep groundwater flow paths cannot penetrate the layer of clay and gyttja which form as sediments in typical low-relief Scandinavian lakes. Flow is anticipated to be directed toward more permeable sediments at the periphery of water bodies and so into the surface water.

Groundwater fluxes in the deeper QD beneath lakes are likely to be slow and diffusion dominated. The results here show that for a zero net flux in the QD there can still be accumulations of radionuclides due to diffusion into the saturated sediments. For iodine there is little difference in upper layer concentrations using the reference K_D values. For radium the assumed value of the Darcy velocity acts to give a higher concentration in the upper layers. The water flux is driving the nuclides through the profile where it is retained.

The reason for the decreasing concentration with increasing Darcy flow is that the loss term from the top of the column carries radionuclides from the upper layer. The situation where there is input to the base of the column (diffusion from the contaminated groundwater in the fracture) into stagnant porewater in the deeper QD is therefore of considerable interest. These results suggest that, even in the case where there is *no water flow* from the fracture to the overburden there can be significant accumulation in the lake sediment.

The situation modelled is relevant for bed sediments but what of the case of wetlands where there may, or may not, be a direct outflow to streams. In situations where evaporation from the soil surface is the mechanism by which standing water is removed from the system there would be no loss of the ^{226}Ra chain members and only loss of iodine would be by volatilisation.

Figure 5-4. Influence of Darcy flow velocity on the equilibrium profile of ^{129}I and ^{226}Ra.

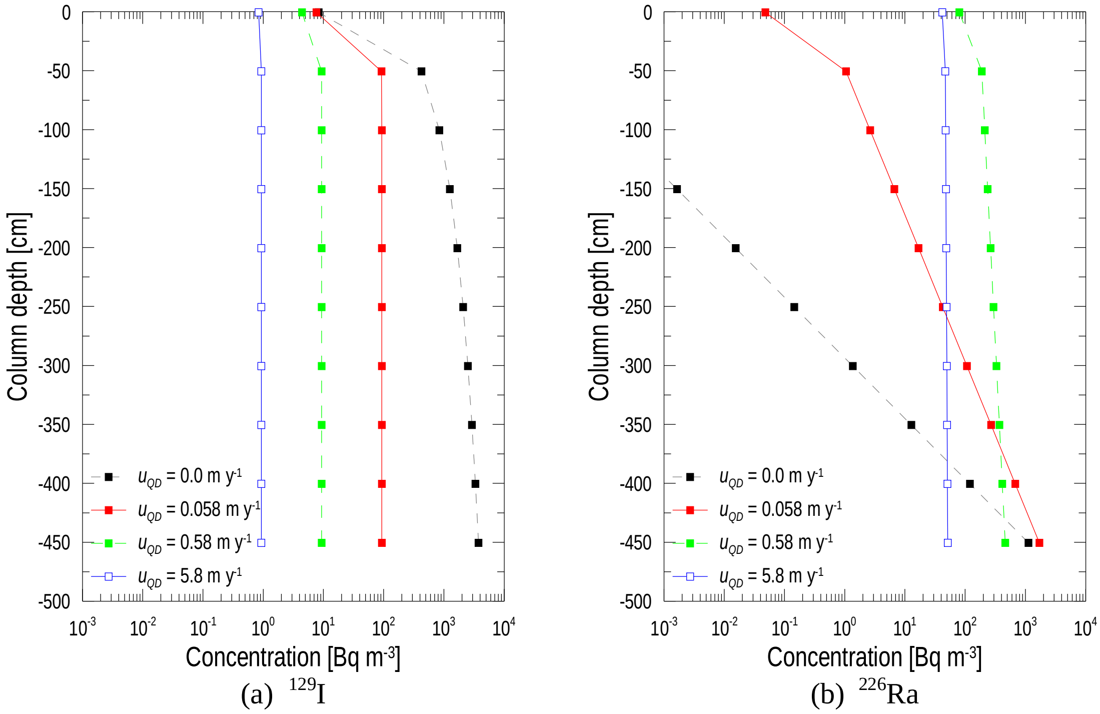


Figure 5-5. Results for the hypothetical evaporative loss case for the alternate K_D dataset.

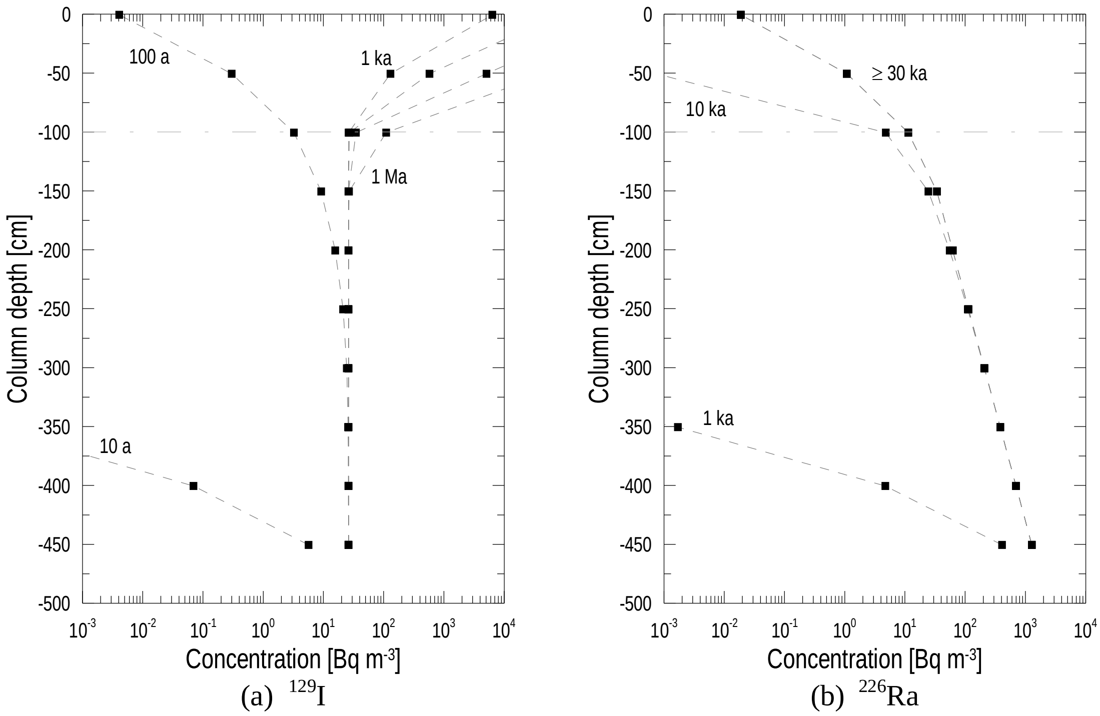


Figure 5-5 illustrates the consequences of evaporative losses for ^{129}I and ^{226}Ra using the alternate K_D dataset. The highly sorbing ^{226}Ra is barely affected by this interpretation of the local hydrology, the equilibrium concentration in the topmost layer increasing by just over an order of magnitude. Again the timescale to equilibrium is around 30 ka.

For ^{129}I the results are quite different in that the though flow of water carries the ^{129}I to the surface where it remains when the solute evaporates. There is continued accumulation in the upper layer over time. However, this is a static interpretation of the landscape object which is unlikely to arise in reality. Nevertheless the result for 1 ka of accumulation suggests that alarmingly high concentration might be possible. This is not a scenario that has been discussed in the hydrology of Forsmark. It may not be possible for contaminated groundwater to approach the surface without dilution. Until the fate of water leaving the bedrock fractures is adequately described it is not possible to rule out such extreme cases, particularly when the spatial extent of the dispersal of contamination is more an issue of the spatial resolution of the model elements rather than being based on physical processes.

6 CONCLUSIONS

The GEMA3D approach is a practical method for modelling extended catchment systems. Numerical results indicate that the surface system close to the release point (ie, along the fracture) is the most important area of the landscape. Early representations of landscape features using a two dimensional array of GEMA3D landscape elements (lels) demonstrated that even weakly sorbing radionuclides remain localised close to the major flow axis of the drainage system, leading to the essentially linear representation of the landscape described here. Streams are therefore a important feature of the landscape to be modelled.

More strongly sorbing radionuclides remain close to the discharge point. Release from fractures in the bedrock are therefore important in the characterisation of the extended biosphere. The lateral spread of radionuclides entering the biosphere is likely to be quite restricted. The key in evaluating radiologic al consequences is therefore to integrate over a representative spatial area. The 10^4 m^2 (1 ha) family farm is suggested for this purpose. Results also support the idea that only agricultural systems are of primary importance in the evaluation of dose since the usage of locally derived foodstuffs can maximise dose on relatively small spatial scales. The amount of net primary production required from natural and semi-natural landscapes is too small leading to large spatial dilution. However, non-agricultural lels can be important *accumulators* of contaminants and so must be included in the assessment model.

Modelling advective transport in the geosphere-biosphere interface has been demonstrated here using the Ecolego transport block. Of primary importance is an adequate representation of local hydrology. At present it is not possible to be sure that the spatial scales discussed in SKB’s SDM 2.3 reports are sufficient to characterise dilution and accumulation in the upper QD. The interpretation of deep groundwater flow from bedrock fractures is essential to the adequate evaluation of dose. For example, it is not possible to rule out the evaporative loss scenario for the geosphere-biosphere interface described here. Such a situation – where standing water above high permeability saturated wetlands is lost by evaporation – could lead to significant doses latent doses. This scenario should be investigated further.

A practical approach to dealing with the dimensions of the biosphere for dose assessments is presented here. Results, in terms of landscape element DCFs, are higher than are to be expected from the SKB modelling approach of the SR-Can vintage. The approach is consistent with the need to calculate dose to a small number of (adult) individuals but avoids the possibility of unrealistically high doses from extreme situations, based on small contaminated areas.

The GEMA3D model is responsive to local conditions and so can be configured for specific areas in the present day biosphere and can also be used to determine the most radiologically important *types* of systems in the future landscape. The size of the object is largely determined by the release fracture and the local topography.

For assessment purposes then, a practical implementation of a reference-biospheres approach has been developed which extends the generic concepts of earlier methodologies to take into account known site conditions. A more practical demonstration will require a reinterpretation of the SDM 2.3 site descriptive models. The database from SR-Can and earlier assessments is no longer sufficient for the detail possible in the GEMA3D which, in turn, expresses relevant detail in the biosphere.

DCFs have been calculated here using the aggregated transfer factors derived by SKB for SR-Can. It would be useful for SSM to derive its own set of corresponding data or to employ a full exposure pathway sub-model.

With respect to wider biosphere modelling issues in long-timescale safety assessments, the issue of the geosphere-biosphere interface emerges, yet again, from the modelling reported here as a primary source of uncertainty in the dose assessment model.

Although fairly simple in the representation of the geosphere-biosphere interface, and at an early stage of development with a considerable amount of detailed information concerning the nature of biosphere objects in the future Forsmark surface environment still to be assimilated into models to be used in the review of SKB's SR-Site assessment, the results from GEMA3D show that a better understanding of the geosphere-biosphere interface is required in respect of the following modelling results:

1. Retention in the deeper QD restricts losses from the system and can allow significant accumulation of radionuclides to build up during periods before the location can be exploited for agricultural usage,
2. Even after the transition to agricultural land concentrations in productive soils can remain for a significant period of time at higher levels than arise under steady state conditions resulting from chronic releases to agricultural systems. Retention, governed by local water fluxes and the chemistry of soils and the deeper QD chemistry can therefore lead to relatively high levels of radiological exposure which exceed those found in the case of chronic releases to agricultural land.
3. The key to understanding the potential for chronic accumulation on the spatial scale of individual farms is the local hydrology. The interaction of deep groundwater transporting radionuclides from the repository to the surface environment and how this mixes with the larger amounts of infiltrating meteoric water is the key issue.

It is known that contaminated groundwater discharges to the QD at the upper expression of the fracture at the bedrock / QD interface. At present there is insufficient detail in the description of these processes. Furthermore, the fractures coincide with local topographic minima and that surface streams are formed in the landscape in broadly aligned with the fracture network at the surface.

The models here have been run until equilibrium is established, assuming a constant release to the bottom of the q-compartment of the model. The dimensions of the landscape elements employed here have been chosen so as to represent areas suitable for radiological assessment. It is not known how long the duration of a release from the bedrock into the biosphere would remain at or near peak levels. It is anticipated that the release from the bedrock will vary in both time and space. From the results presented here the time during which the release remains within the boundaries of any particular landscape element is important. The shape of the contaminant plume is therefore required for an adequate description of the geosphere-biosphere interface. A narrow, rapidly moving profile would not have sufficient time to build up significant accumulations in the biosphere objects, a broad, slow moving plume might.

Given the significance of accumulation, the potential of eskers and related features assume a greater importance than hitherto. Their dynamics and longevity, coupled to the description of the contaminant plume should be investigated in future model descriptions.

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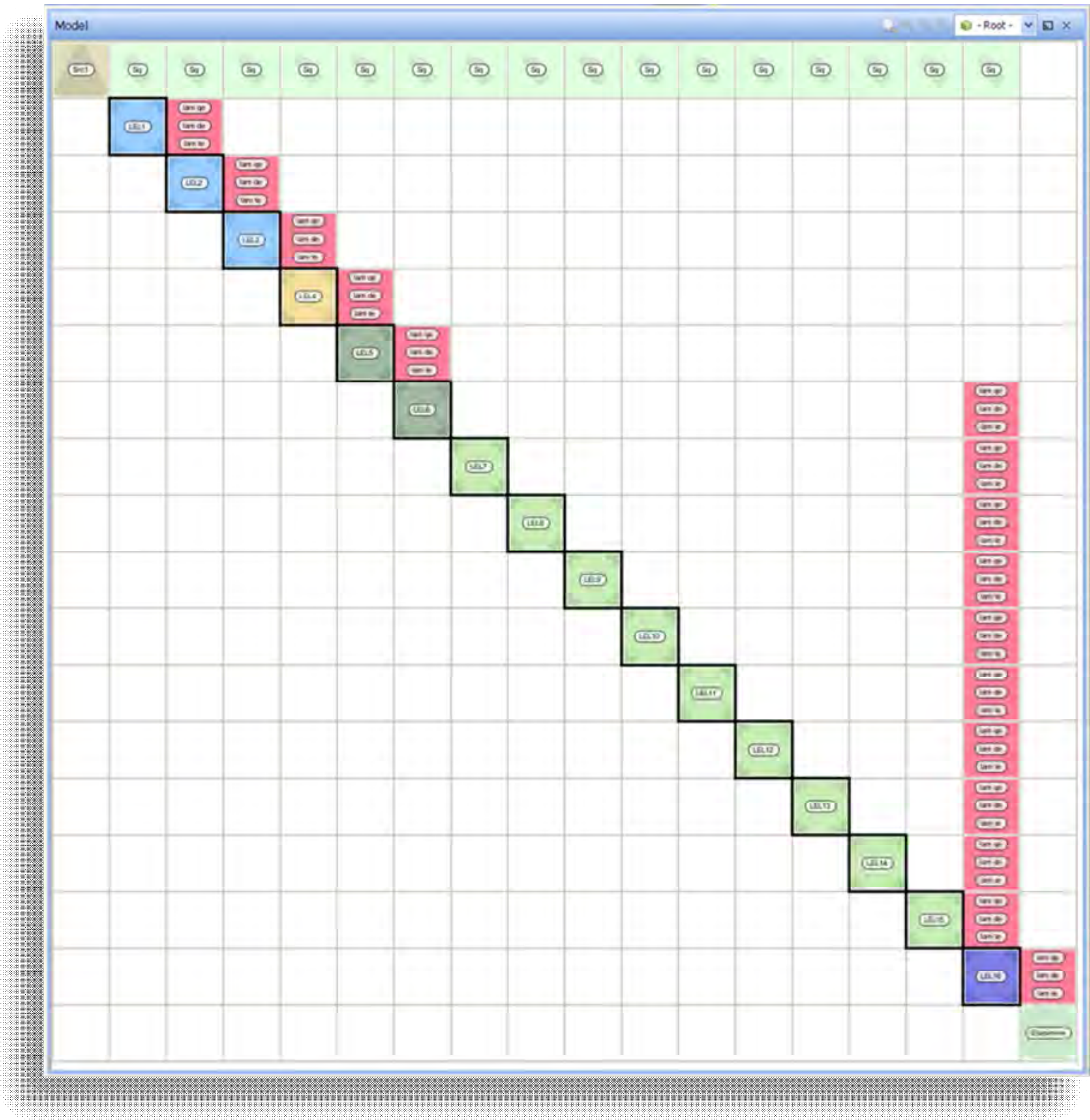
APPENDIX A – IMPLEMENTATION IN ECOLEGO

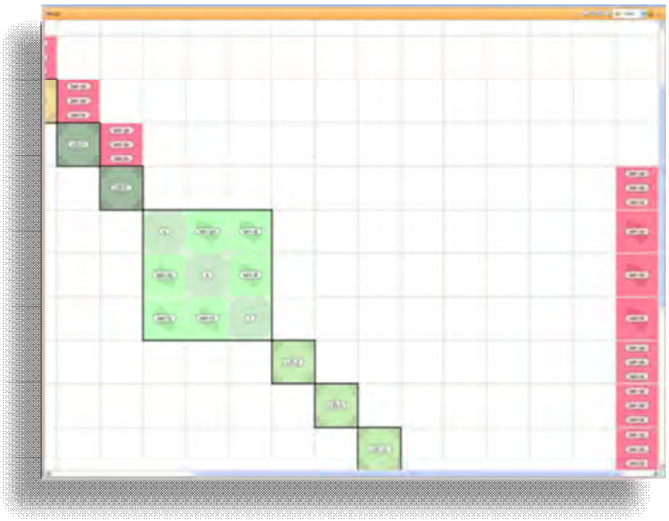
Overall system

The Ecolego GUI has proved to be very useful in setting up the model of the sixteen landscape elements. In this image from the model the leading diagonal contains the sixteen lels and the off-diagonal indicates the inter-lel transfers. As modelled the lake (lels 1 - 3) flows into the wetland (lel4), which flows (as an aquifer) beneath the forest (lels 5 & 6) before discharging to the stream (lel16). Each of the agricultural lels (7 – 15). Each of the agricultural lels discharges to the aquifer under the stream. Irrigation takes place in lels 7 and 15 but, as an internal process to the lels themselves, is not depicted here.



Internal landscape element

Inside each of the lel sub-models the transfer coefficients are defined using Equation (A.1) for each internal compartment and each external transfer. The water and solid material fluxes are defined as follows:



lel7 - irrigated agricultural land

Water fluxes

	FAt	$m^3\ y^{-1}$	A*(ppt-ETp)	net precipitation
	FCd	$m^3\ y^{-1}$	0	source to d-
	FCq	$m^3\ y^{-1}$	FSq*sqrt(A)*wf	source to q-
	FCt	$m^3\ y^{-1}$	0	source to t-
	Fjd	$m^3\ y^{-1}$	0	inflow from other lels
	Fjq	$m^3\ y^{-1}$	0	
	Fjt	$m^3\ y^{-1}$	0	
Internal fluxes	Fde	$m^3\ y^{-1}$	0	
	Fdq	$m^3\ y^{-1}$	Ftd+Fqd-Fdt	
	Fdt	$m^3\ y^{-1}$	capil_rd*A	
	Fqd	$m^3\ y^{-1}$	capil_rq*A	
	Fqe	$m^3\ y^{-1}$	Fdq+Ftq-Fqd-Fqt+Fjq	
	Fqt	$m^3\ y^{-1}$	d_irri*A	
	Ftd	$m^3\ y^{-1}$	Fdt+FAt+Fqt	
	Fte	$m^3\ y^{-1}$	0	
	Ftq	$m^3\ y^{-1}$	0	

Solid material fluxes

External fluxes	MAt	$kg\ y^{-1}$	0	net deposition
	MCd	$kg\ y^{-1}$	0	source to d-
	MCq	$kg\ y^{-1}$	0	source to q-
	MCt	$kg\ y^{-1}$	0	source to t-
	Mjd	$kg\ y^{-1}$	0	inflow from other lels
	Mjq	$kg\ y^{-1}$	0	
	Mjt	$kg\ y^{-1}$	0	
Internal fluxes	Mde	$kg\ y^{-1}$	0	
	Mdq	$kg\ y^{-1}$	Mqd+Mtd-Mdt	
	Mdt	$kg\ y^{-1}$	wd*md*A+Fdt*alphaq	
	Mqd	$kg\ y^{-1}$	Fqd*alphaq	
	Mqe	$kg\ y^{-1}$	0	
	Mqt	$kg\ y^{-1}$	Fqt*alphaq	
	Mtd	$kg\ y^{-1}$	(mdep-me)*A+Mdt+Mqt	
	Mte	$kg\ y^{-1}$	0	
	Mtq	$kg\ y^{-1}$	0	

The water and solid material fluxes are written in terms of model parameters (see Appendix C) for defined fluxes and other fluxes to account for mass balance. For the irrigated land the irrigation parameter (d_irri) is non zero, providing a water flux from the q-compartment directly to the top soil. Suspended particulates in the porewater contribute a small solid material flux.

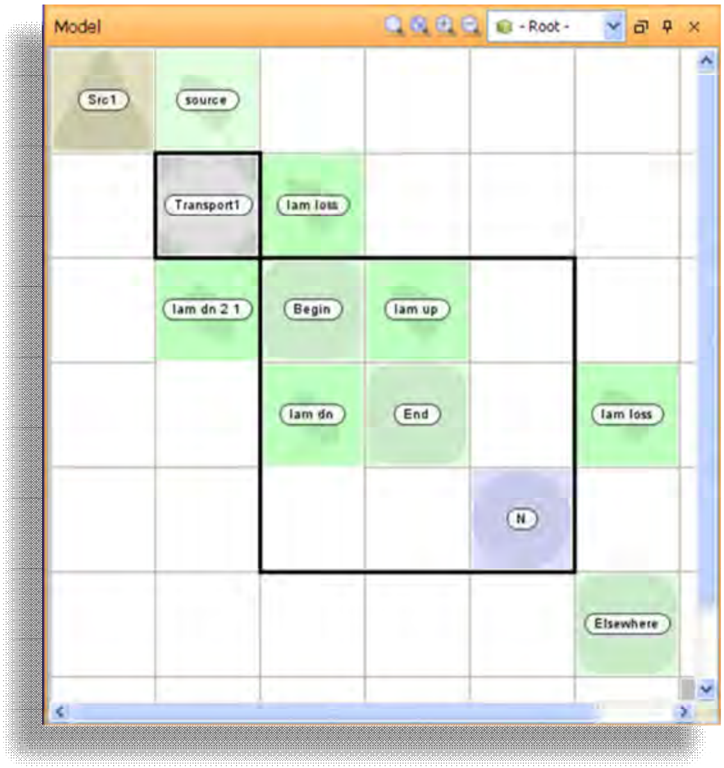
Linkages between the Ecolego sub-models are need to propagate the flow of contaminants through the drainage system. The stream provides the most dramatic example of this with inputs from all nine agricultural lels as well as from the forest. The water fluxes for lel16 the stream are:

lel16 - drainage stream

Water fluxes				
	FAt	$m^3\ y^{-1}$	A*(ppt-ETp)	net precipitation
	FCd	$m^3\ y^{-1}$	0	source to d-
	FCq	$m^3\ y^{-1}$	0	source to q-
	FCt	$m^3\ y^{-1}$	0	source to t-
	Fjd	$m^3\ y^{-1}$	0	
	Fjq	$m^3\ y^{-1}$	LEL6.Fde + LEL7.Fqe + LEL8.Fqe + LEL9.Fqe + LEL10.Fqe + LEL11.Fqe + LEL12.Fqe + LEL13.Fqe + LEL14.Fqe + LEL15.Fqe	inflow from other lels
	Fjt	$m^3\ y^{-1}$	0	
Internal fluxes	Fde	$m^3\ y^{-1}$	0	
	Fdq	$m^3\ y^{-1}$	0	
	Fdt	$m^3\ y^{-1}$	Fqd	
	Fqd	$m^3\ y^{-1}$	Fjq	
	Fqe	$m^3\ y^{-1}$	0	
	Fqt	$m^3\ y^{-1}$	0	
	Ftd	$m^3\ y^{-1}$	0	
	Fte	$m^3\ y^{-1}$	Fdt+FAt+Fjt	
	Ftq	$m^3\ y^{-1}$	0	
Solid material fluxes				
External fluxes	MAt	$kg\ y^{-1}$	0	net deposition
	MCd	$kg\ y^{-1}$	0	source to d-
	MCq	$kg\ y^{-1}$	0	source to q-
	MCt	$kg\ y^{-1}$	0	source to t-
	Mjd	$kg\ y^{-1}$	0	
	Mjq	$kg\ y^{-1}$	LEL6.Mde + LEL7.Mqe + LEL8.Mqe + LEL9.Mqe + LEL10.Mqe + LEL11.Mqe + LEL12.Mqe + LEL13.Mqe + LEL14.Mqe + LEL15.Mqe	inflow from other lels
	Mjt	$kg\ y^{-1}$	0	
Internal fluxes	Mde	$kg\ y^{-1}$	0	
	Mdq	$kg\ y^{-1}$	0	
	Mdt	$kg\ y^{-1}$	Mqd	
	Mqd	$kg\ y^{-1}$	Mjq	
	Mqe	$kg\ y^{-1}$	0	
	Mqt	$kg\ y^{-1}$	0	
	Mtd	$kg\ y^{-1}$	mdep*A	
	Mte	$kg\ y^{-1}$	Mdt	
	Mtq	$kg\ y^{-1}$	0	

APPENDIX B – MODEL OF A QD COLUMN

Implementation of a transport block in Ecolego is simple. A two domain block is illustrated:



The first block is shown collapsed and the second is expanded to illustrate the lower (Begin) and upper (End) compartments. The transfer coefficients are defined to be the same for all parts of the block. The number of compartments in the block is denoted by the "block" *N*. The Equations are

$$\lambda_{up} = \frac{v_{QD}}{R_{QD} l_{QD}} + \frac{D}{R_{QD} l_{QD}^2} \ \mathrm{a}^{-1}, \qquad \text{(C.1)}$$

$$\lambda_{down} = \frac{D}{R_{QD} l_{QD}^2} \ \mathrm{a}^{-1}, \qquad \text{(C.2)}$$

which is also valid for the loss term.

The retardation factor for each compartment in the block is

$$R_{QD} = \theta_{QD} + (1 - \varepsilon_{QD}) \rho_{QD} k_{QD} \ \text{-}. \qquad \text{(C.3)}$$

The internal parameters for the block are:

Parameter	Value	Units	Block	Description
D	0.0127	$m^2\ y^{-1}$	Transport2	diffusion constant
epsQ	0.3	-	Transport2	porosity of QD
KD	0.0	$m3\ kg^{-1}$	Transport2	Solid-liquid distribution coefficient QD
L	1.0	m	Transport2	Thickness of QD
rho	2650.0	$kg\ m^{-3}$	Transport2	Grain density
uDarcy	0.058	$m\ y^{-1}$	Transport2	Darcy velocity

The up and down transfers between blocks are written in the same way as for the internal transfers. In this way advective-dispersive transport between layers with different properties can be modelled.

The full description of the block equations for this two layer example is:

block	Expression	sub-model
source	0	
Src1		
Begin	0	Transport1
Cbeg	Begin/(L/D)	Transport1
Cend	End/(L/N)	Transport1
End	0	Transport1
lam_dn	D/R/(L/N)^2.0	Transport1
lam_loss	uDarcy/R/(L/N)+D/R/(L/N)^2.0	Transport1
lam_up	uDarcy/R/(L/N)+D/R/(L/N)^2.0	Transport1
N	60	Transport1
R	epsQ+(1.0-epsQ)*rho*KD	Transport1
Begin	0	Transport2
Cbeg	Begin/(L/D)	Transport2
Cend	End/(L/N)	Transport2
End	0	Transport2
lam_dn	D/R/(L/N)^2.0	Transport2
lam_dn_2_1	D/R/(L/N)^2.0	Transport2
lam_loss	uDarcy/R/(L/N)+D/R/(L/N)^2.0	Transport2
lam_up	uDarcy/R/(L/N)+D/R/(L/N)^2.0	Transport2
N	50	Transport2
R	epsQ+(1.0-epsQ)*rho*KD	Transport2
Elsewhere	0	

The system easily extended to multiple transport blocks as described in Chapter 5.

APPENDIX C – DATABASE FOR THE GEMA3D EXAMPLE SYSTEM

Name	Iel	Value	Units	Description
A10Agri	-	8470	m^2	Area of ecosystem as lake required to support 10 adults agricultural ecosystems
A10FW	-	1220000	m^2	Area of ecosystem as lake required to support 10 adults freshwater ecosystems
A10Nat	-	3660000	m^2	Area of ecosystem as lake required to support 10 adults natural ecosystems
wf	-	0.0002	m	fracture half width
A	16	10000	m^2	Iel area
	1 to 15	10000		
Acatch	1 to 3	30000	m^2	local catchment area
	4 to 16	0		
alphad	1 to 16	0.001	kg m^{-3}	suspended solids in d-compartment
alphaq	1 to 16	0.001	kg m^{-3}	suspended solids in q-compartment
alphat	1 to 16	0.001	kg m^{-3}	suspended solids in t-compartment
capil_rd	1 to 6, 16	0	m a^{-1}	capillary rise from d-compartment
	7 to 15	0.4		
capil_rq	1 to 6, 16	0	m a^{-1}	capillary rise from d-compartment
	7 to 15	0.4		
d_irri	1 to 6, 8 to 14, 16	0	m a^{-1}	irrigation rate
	7, 15	0.15		
D0	D0	0	m^2 a^{-1}	diffusion constant
epsd	1 to 16	0.3	-	porosity d-compartment
epsq	1 to 16	0.3	-	porosity q-compartment
epst	1 to 3, 16	1	-	porosity t-compartment
	5, 6	0.3		
	4, 7 to 15	0.5		
ETp	1 to 16	0.4	m a^{-1}	ETp

Name	Iel	Value	Units	Description
FSq	1 to 15	0.0058	$m^3\ a^{-1}$	Water flux from fracture
ld	1 to 4, 16	0.1	m	thickness d-compartment
	5 to 15	0.3		
lq	1 to 4 - 16	0.9	m	thickness q-compartment
	5, 6	0.5		
	7 to 15	0.4		
lt	1 to 3	1	m	thickness t-compartment
	4, 15	0.5		
	5, 15	0.3		
md	1 to 5, 16	0	$kg\ m^{-2}$	Active biomass in d-compartment
	6 to 15	0.1		
mdep	1 to 16	0	$kg\ m^{-3}\ a^{-1}$	Local deposition rate
me	1 to 16	0	$kg\ m^{-3}\ a^{-1}$	Local erosion rate
ppt	1 to 16	0.6	$m\ a^{-1}$	Local precipitation
rhod	1 to 16	2650	$kg\ m^{-3}$	grain density d-compartment
rhoq	1 to 16	2650	$kg\ m^{-3}$	
rhot	1 to 16	2650	$kg\ m^{-3}$	
rhoW	1 - 16	1000	$kg\ m^{-3}$	standard density of water
thetad	1 to 6, 16	0.3	-	volumetric moisture content d-compartment
	7 to 15	0.2		
thetaq	1 to 15	0.3	-	volumetric moisture content q-compartment
	16	0.5		
thetat	1 to 3, 16	1	-	volumetric moisture content t-compartment
	4	0.5		
	5, 6	0.2		
	7 to 15	0.3		
wd	1 to 4, 16	0	a^{-1}	Biomass activity (times per year)
	5 to 15	20		

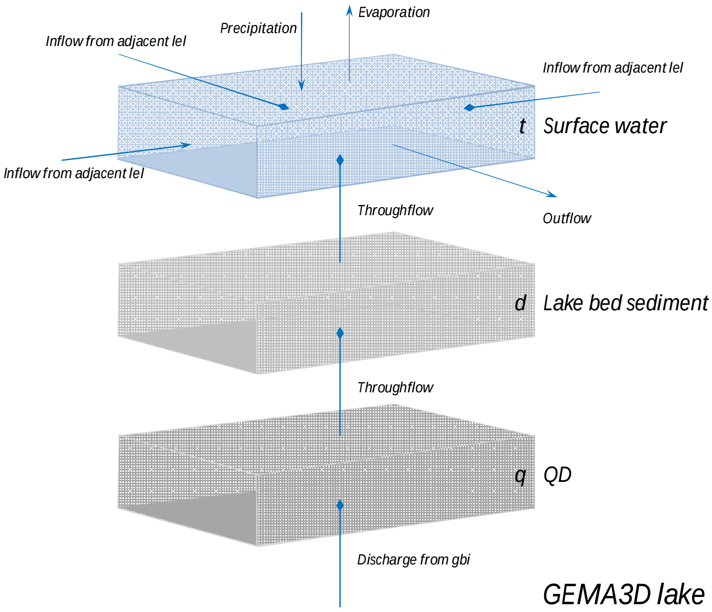
Name	Nuclide	Value	Units	Description
aDust	-	0.0001	kg dw m^{-3}	airborne dust load
Icarbon	-	110	kgC y^{-1}	Carbon consumption rate
Idw	-	0.6	m^3 y^{-1}	ICRP Ref Man
Iinh	-	8020	m^3 y^{-1}	Nagra NIB 02-001 - the TAME value!
Occf	-	1	y y^{-1}	lel occupancy factor - full occupancy
G	I-129	0.0	(Sv y^{-1}) (Bq m^{-3} ww)$^{-1}$	External exposure factor
	Ra-226	6E-16		
	Pb-210	7.2E-17		
	Po-210	0		
Hing	I-129	1.10E-07	Sv Bq^{-1}	Dose per unit intake - ingestion
	Ra-226	2.80E-07		
	Pb-210	6.90E-07		
	Po-210	1.20E-06		
Hinh	I-129	3.60E-08	Sv Bq^{-1}	Dose per unit intake - inhalation
	Ra-226	9.50E-06		
	Pb-210	5.60E-06		
	Po-210	4.30E-06		

Name	Nuclide	Value	Units	Description
TFagg_agri	I-129	0.72	(Bq kgC^{-1}) (Bq kg^{-1} dw)	TFagg for agricultural ecosystems
	Ra-226	0.04		
	Pb-210	0.021		
	Po-210	0.025		
TFagg_fw	I-129	0.073	(Bq kgC^{-1})(Bq $m^{-3})^{-1}$	TFagg for freshwater ecosystems
	Ra-226	22		
	Pb-210	0.036		
	Po-210	0.15		
TFagg_irri	I-129	0.054	(Bq kgC^{-1})(Bq $m^{-3})^{-1}$	TFagg for irrigated ecosystems
	Ra-226	0.032		
	Pb-210	0.028		
	Po-210	0.028		
TFagg_natSoil	I-129	4	(Bq kgC^{-1}) (Bq kg^{-1} dw)	TFagg for natural ecosystems
	Ra-226	7.4		
	Pb-210	0.01		
	Po-210	0.52		

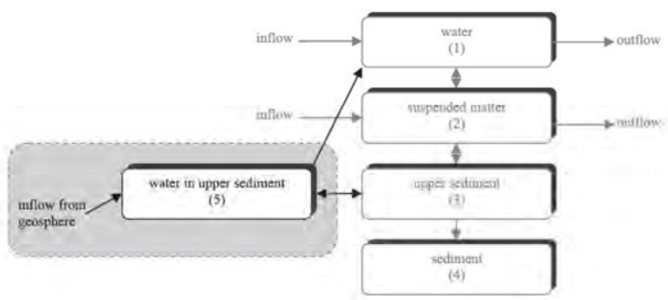
APPENDIX D – COMPARISON OF GENERIC HYDROLOGICAL REPRESENTATIONS FOR DIFFERENT ECOSYSTEMS WITH CORRESPONDING SKB MODELS

This appendix illustrates the conceptual differences between the GEMA3D lels implemented here and their SKB counterparts taken from SKB (2006a) and Bergström *et al*. (2008) for SR-Can and SAR-08 respectively. NB, in SAR-08 the mire and forest models were the same. Streams were not modelled by SKB. It is expected that SKB's models for SR-Site will be revised.

Lake model:



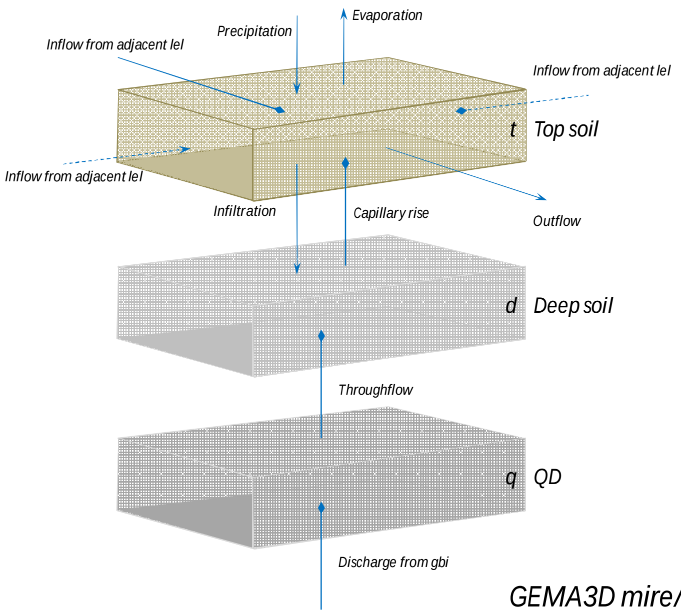
GEMA3D lake (bay) lel



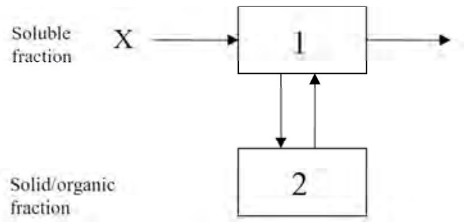
SKB 's coastal and lake model

The main difference are: 1. that radionuclides in the GEMA3D model interact with deeper sediments, leading to greater potential retention in the modelled lel. 2. The GEMA3D model is an *element* of the whole lake whereas the SKB model *is* the whole lake, giving greater volumetric dilution.

Mire/forest model:



GEMA3D mire/forest lel



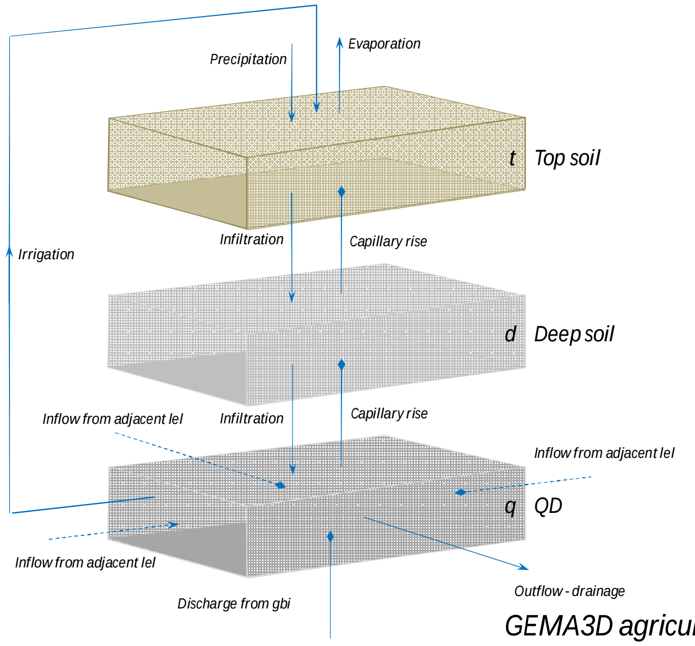
SKB 's mire/forest model

The GEMA3D model treats the mire as a component of the surface system with input from below, allowing for greater retention. There can be input from into the upper (t-) layer where the main water flux is seen as flowing water from the adjacent lake system. Aside from the deeper accumulation in the GEMA3D interpretation, both models assume the greatest water flux is through the upper layer of the wetland. The SKB distinction between soluble and solid phases can be straightforwardly modelled used the k_d concept.

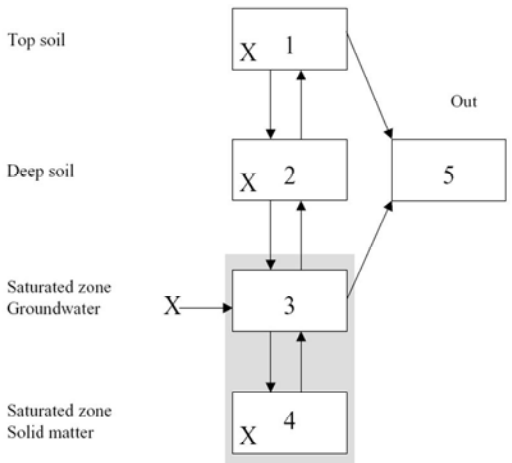
In SAR-08 SKB used their mire model to represent forested areas. This is reasonable since the focus was on long term accumulation. The forest interpretation in GEMA3D makes a similar assumption.

As with the lake model, the GEMA3D lel is the *contaminated* part of the mire allowing for the localisation of contaminants. In the earlier SKB approach the mire represented the whole of the mire ecosystem.

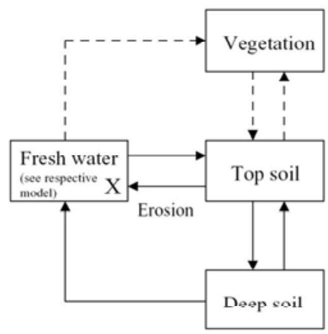
Agricultural / irrigated land model:



GEMA3D agricultural lel



SKB 's agricultural land model

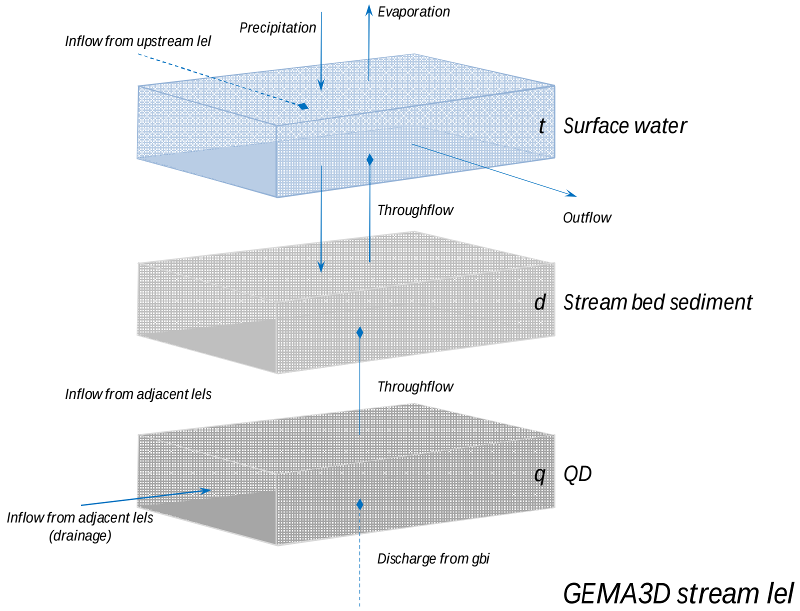


Structure of the sub-model irrigation

Dynamic transfers are shown with solid arrows, equilibrium by dashed arrows

The agricultural land models are similar in construction – the distinct water and solid compartments of SKB's agricultural land can be modelled using the k_d concept as a single compartment. Areas of land are again an issue, the reasoning behind the use of a 1 ha lel for agricultural land in GEMA3D is discussed in the main text. The GEMA3D model integrates agricultural land with the irrigation model. The main difference is that SKB's model anticipates irrigation from fresh water (usually a lake with high dilution) whereas in the model described here an aquifer in the QD is assumed to serve this purpose. Well water is therefore assumed to be extracted and applied to the t-compartment where it percolates through the soil column, back to the QD. Stream water could be used as an alternative but this is likely to be at greater dilution so the higher concentration in the QD aquifer are employed as a conservative assumption.

Stream model:



Although SKB have developed a specific stream model it has not been used to calculate doses. This simple model assume direct input through the QD aquifer, including drainage water from the adjacent managed farmland. Xu *et al*. (2008) suggest a rather more detailed interpretation with increased interaction between water column and bed sediments.

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