

2002:22 RICHARD KLOS

Review of data types for the SKB site investigation programme



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TITLE/TITEL: Review of data types for the SKB site investigation programme/ Behov av data från en platsundersökning: Översikt och synpunkter på SKB:s platsundersökningsprogram.

SUMMARY: SKB is currently undertaking a detailed site investigation programme (SIP) to characterise the geology and surface ecosystems in areas around potential sites for a planned repository for spent nuclear fuel.

This report reviews site specific and generic data types needed to characterise biosphere processes relevant to the evaluation of long-term radiological safety in the context of assessments of future impacts arising from the deep geologic disposal of spent nuclear fuel. Focus is on the types of data that make up the different elements of radiological assessment models and how the data used relate to site-specific characteristics. The relevance of the SIP to the development of assessment models for long-term assessment is addressed, including the representation of the geospherebiosphere interface.

Reference to SKB's programme is made in order to determine how well the current programme will meet the needs of assessment models that will be developed and used in the assessment of long-term safety. The review also provides SSI with a basis for the planning of further SSI R&D work.

The process, by which site-specific information is converted into a form suitable for use in numerical assessment models, can be quite complex. An overview of assessment model concepts is provided and the links between these and real-word site information considered. Focusing on the needs of assessment models, the review provides a summary of the main types of analyses and site-specific models that are needed for safety evaluations.

Review of the SIP indicates that information from the programme feeds into a set of detailed site description models. However there is a gap between the descriptive components and the detailed model descriptions needed to configure numerical assessment models. Details of system evolution are not clearly dealt with in the programme. The SIP focuses on a detailed description of the site the present day. However, radiological impacts are not expected to reach their peak until far into the future. It is not yet apparent how SKB will use SIP information in the representation of the biosphere system at future times.

It is concluded that the SIP addresses the right kind of entities to allow radiological assessment models to be defined. However it is suggested that a change of emphasis be introduced, so as to focus more on the driving forces for contaminant bearing material fluxes rather than on turnover times. This means that more attention should be paid to the physical transport processes, integrating existing details of the different ecosystems relevant to Swedish conditions. Developments of assessment modelling capability should consider the need to include a more spatially extended assessment model representation than has been the case so far in radiological assessments.

SAMMANFATTNING: SKB genomför för närvarande platsundersökningar som syftar till att karakterisera geologi och ytnära ekosystem på möjliga platser för det planerade slutförvaret för använt kärnbränsle.

Denna rapport går igenom de platsspecifika och generiska data som behövs för att beskriva de processer i biosfären som är relevanta för analyser av slutförvarets framtida radiologiska skyddsförmåga. Rapporten fokuserar på de data som ingår i de radiologiska konsekvensmodellerna och hur dessa data relaterar till platsspecifika egenskaper. Vidare diskuteras vilka krav som bör ställas på platsundersökningarna, inklusive karakteriseringen av övergången mellan geosfär och biosfär, med hänsyn till behoven av att utveckla modeller för säkerhetsanalysen, och i vilken utsträckning SKB:s platsundersökningsprogram är anpassat för att möta dessa behov. Rapporten SSI rapport : 2002:22 november 2002 ISSN 0282-4434 syftar också till att ge SSI ett underlag för dess fortsatta planering av forskning kring platsundersökningar.

Processen att överföra information och data från en plats till ett lämpligt format för numeriska beräkningsmodeller kan vara komplex. Rapporten ger en översikt av de viktigaste analyserna och platsspecifika modellerna som behövs för utvärderingen av förvarets långsiktiga skyddsförmåga, och beskriver hur dessa relaterar till verkliga platsdata.

SKB:s platsundersökningsprogram bedöms vara ändamålsenligt för framtagandet av olika typer av platsbeskrivande modeller, men det finns ett gap mellan de kvalitativa beskrivningarna och den detaljinformation som behövs för att konfigurera de numeriska beräkningsmodellerna. Vidare finns det oklarheter i hur SKB hanterar frågor kring den framtida utvecklingen av biosfären. SKB:s platsundersökningsprogram syftar i första hand till att ta fram en detaljerad beskrivning av dagens förhållanden vid platsen. De största radiologiska konsekvenserna förväntas dock inte uppträda förrän långt in i framtiden. Det är ännu inte klart hur SKB avser att använda informationen från platsundersökningarna för att beskriva framtida biosfärer.

Den övergripande slutsatsen från denna granskning är att SKB:s platsundersökningar kan förväntas ge rätt typ av information för framtagandet av modeller för den radiologiska konsekvensanalysen. SKB rekommenderas dock att lägga större tonvikt på att bestämma drivkrafter för transport av kontaminerat material i förhållande till omsättningstider. Detta innebär att större uppmärksamhet bör läggas på fysiska transportprocesser och deras beskrivning i olika ekosystem som är relevanta för svenska förhållanden. I det fortsatta utvecklingsarbetet med konsekvensmodeller bör SKB även överväga att ta fram rumsligt mer heltäckande modellbeskrivningar jämfört med tidigare analyser.

> Författarna svarar själva för innehållet i rapporten.

The conclusions and viewpoints presented in the report are those of the author an do not necessarily coincide with those of the SSI.



Förord

Statens strålskyddsinstitut (SSI) har till uppgift att bedöma om ett slutförvar för använt kärnbränsle kan uppfylla de krav på skydd av människors hälsa och miljön som ställs i strålskyddslagen (1988:220) och i SSI:s föreskrifter (t.ex. SSI FS1998:1). Svensk Kärnbränslehantering AB (SKB) påbörjade under 2002 platsundersökningar för lokalisering av ett slutförvar i tre områden i Östhammars och Oskarshamns kommuner. Resultaten från dessa platsundersökningar kommer att utgöra ett viktigt underlag i SKB:s ansökan om att få påbörja bygge av ett slutförvar på en plats. Enligt SKB:s nuvarande tidsplaner kommer en sådan ansökan att inges under senare delen av 2007.

SSI driver ett målinriktat forskningsprogram med syfte att vidareutveckla den kompetens och de granskningsverktyg som behövs för att kunna göra kvalificerade granskningar och bedömningar av SKB:s arbete med slutförvaring av kärnavfall. Det forskningsprojekt som redovisas i denna rapport utgör en sammanställning av data och modeller som behöver tas fram under en platsundersökning för att kunna genomföra analyser av slutförvarets långsiktiga skyddsförmåga. Vidare kommenteras översiktligt omfattning och inriktning på SKB:s redovisade program för karakterisering av biosfären, inklusive kvartära avlagringar och de övre delarna av geosfären. Resultaten från detta projekt kommer att användas som ett av flera underlag för planeringen av SSI:s fortsatta forskning inom området platsundersökningar.

Arbetet har utförts av Ryk Klos vid konsultföretaget Galson Sciences Ltd i England, på uppdrag av Björn Dverstorp, avdelningen för avfall och miljö. Författaren svarar själv för innehållet i denna rapport.

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APPENDIX A The role of solid material transport in the terrestrial biosphere

1 Introduction and objectives

Over the past few years there have been significant developments in the content of biosphere models used in SKB's performance assessments (PAs) of Swedish radioactive waste disposal options. SKB's current model configurations require a large amount of data to support and match their potential capabilities.

The aims of this project are:

- to provide the Swedish regulators (SSI) with a compilation of relevant site-specific and generic biosphere data types, including data for the geosphere-biosphere interface, that will be needed to develop an understanding of biosphere processes relevant for evaluation of long-term safety and radiological protection;
- to summarise the main types of analyses and site-specific models that are needed for the safety evaluation;
- to assess how well SKB's programme meets the above needs, to identify any major gaps in SKB's programme in relation to SSI's regulations or international experience, to assess whether the timing of various measurements is appropriate; and
- to provide a base document for SSI's future work on biosphere characterisation, i.e. for review of SKB's site investigation programme and for the planning of further SSI R&D work.

The aims are addressed in the three work areas described below.

Summary of data types

Based on experience in the Swiss assessment programme [e.g., Kłos *et al.*, 1996], the work of BIOMOVS II [1996] and BIOMASS [IAEA, 2001a], as well as elements from the BNFL [2000] and UK Nirex [1997] approaches to biosphere modelling, a review of the components of biosphere assessment models for long-term radiological assessment has been carried out. Reference to biosphere modelling in Project SAFE is also made [Kłos and Wilmot, 2002].

Focus is on the types of data that make up the different elements of radiological assessment models and how the data used relate to site-specific characteristics. The characterisation and representation of the geosphere-biosphere interface is included. The review takes into account the current plans of SKB for the characterisation of the biosphere in Sweden within the spent fuel disposal programme [specifically SKB, 2000; SKB, 2001a; SKB, 2001b]. The current approach to biosphere assessment modelling in Sweden has also been reviewed, in particular the representation of the Forsmark site [SKB, 2001c]. The context for the review is set by the guidance of SSI [2000].

Review of necessary site-specific analysis and models

Like data, models used in PA may themselves show varying degrees of site specificity. There is often a hierarchy of models used in the definition of the numerical assessment model ultimately used in the PA calculations since site characterisation data are not usually directly usable in PA models. A phase of interpretation and pre-processing is required. The review considers those site characteristics that can be observed and measured as part of a site investigation programme

and the methods and models by which these are translated into usable entities within the numerical assessment model.

Preliminary review of SKB's biosphere site characterisation programme for spent fuel disposal The review addresses the following points:

- Are the right entities to be characterised?
- What is the corresponding numerical assessment model entity and how are the supporting model data and the assessment quantity related?
- Is the interpretation of measured/observed data correct (taking into account how information may be traced through the system and model identification, justification and description stages)?
- What is the scope of the numerical assessment model data (spatio-temporal, nuclide, chemical boundary conditions – range of applicability within the numerical assessment model)?

The review also includes discussion of how biosphere characterisation and assessment have been handled in a few other selected radioactive waste disposal programmes (NAGRA in Switzerland, and Nirex and BNFL in the UK), to provide a view on the relative state of advancement of SKB's biosphere programme

2 Summary of data types

2.1 Background

A primary aim of this project is to provide SSI with a review of the relevant types of data for use in the assessment of radiological impact and to discuss the needs of the assessment in terms of the site investigation programme (SIP) being carried out by SKB in support of a license application for the construction of a deep repository for spent fuel from the Swedish Nuclear Power Programme.

Performance assessments of this kind have been carried out over several years by SKB and there is a wealth of background material and experience in the definition and application of longterm assessment models. Nevertheless, although the broad outlines of the models to be used are well established, the details of the actual models themselves (in terms of the geographic areas, and evolutionary trends) are not yet finally established. It is also likely that when the sites investigated are fully characterised, model details may include some feature, events and processes (FEPs) not yet incorporated in the modelling work carried out to date.

It is still unclear which models and codes SKB will use as a basis for the license application. However, various sub-models are already in existence and, together with the experience of other similar programmes, it is possible to determine the kinds of systems and sub-systems which are likely to be employed in PA modelling. In order to characterise the types of data required for assessment of long-term radiological impact, experience from elsewhere will be used [Kłos *et al.*, 1996; BIOMOVS II, 1996; Nirex, 1997; BNFL, 2000; IAEA, 2001a] as well as direct reference to recent SKB biosphere modelling effort [Karlsson *et al.*, 2001; SKB, 2001c] and reviews thereof [Kłos and Wilmot, 2002].

2.2 Requirements of assessment models

Ultimately, long-term radiological safety must be judged, at least in part, by the application of numerical assessment models and the interpretation of their results. The purpose of the model is to evaluate the potential health impact of the release of radionuclides from the repository to the biosphere¹. Numerical assessment models, and the data used with them, are the primary focus of this review of data types. At this stage it is useful to review the composition of such models.

Numerical assessment models must include representations of:

- inputs of radionuclides to the system;
- transport of contaminants within the system;
- accumulation of contaminants in components of the system;
- exposure (risk/dose) of selected groups to environmental concentrations of contaminants in the system; and
- losses of contaminants from the modelled system.

¹ For the purposes of this review, the 'biosphere' is taken to include all aspects of the geosphere-biosphere interface.

It is important to recognise that, in the biosphere component of the overall PA model system, concentrations of radionuclides are likely to be low enough that the model should represent the system as it would be in the absence of contaminants. All FEPs modelled should be those at work whether or not radionuclides have been released into the system. In this way the focus shifts to the FEPs acting to move material around the system. Movement of material drives the transport of contaminants.

In general, material flows may be characterised as water and solid material fluxes [Kłos *et al.*, 1996; BIOMOVS II, 1996]. Recent work by SKB [Kumblad, 1999] has focused on the representation of ecosystems. Although attention has been on transport of ¹⁴C, movements of biota containing contaminants in trace quantities may be possible. Ecosystem modelling of biotic movements may therefore play a role in a more generalised description of radionuclide transport [cf. detritus flows in BIOMASS ERB2B: IAEA, 2001]. Gaseous-phase transport is also a possibility but release of radionuclides in groundwater across the geosphere-biosphere interface means that the main focus will be on water solids and organic carbon movements. Nonetheless, the need to develop gaseous-phase transport and accumulation models cannot be ruled out at this stage.

On the basis of current practice, it seems likely that the numerical models will be based on firstorder linear dynamics using a compartment-model approach. The rate of transfer of radionuclide N between compartments i and j is defined by the fractional transfer rate from compartment i to compartment j:

$$\lambda_{ij} = \frac{\text{amount of } N \text{ moved from } i \text{ to } j \text{ in unit time}}{\text{total amount of } N \text{ in compartment } i} = \frac{N_{ij}}{N_i}.$$
(1)

Transfers are mediated by:

 F_{ii} [m³ a⁻¹] water fluxes;

 M_{ii} [kg a⁻¹] solid material fluxes;

 C_{ii} [kg a⁻¹] organic carbon fluxes; and

 G_{ii} [m³ a⁻¹] gaseous fluxes.

The distribution between these phases and the amount retained (accumulated) in compartment *i* is determined by the internal properties of the compartment (the *k* parameters defining them: P_i^k). In general terms, the fractional transfer rates are a function of all of these factors:

$$\lambda_{ij} = f(F_{ij}, M_{ij}, C_{ij}, G_{ij}, P_i^k) y^{-1}.$$
(2)

Written in this way, the task of defining assessment models is to identify the driving forces responsible for material transfer between compartments and then to determine how much of the internal content moves with each of the flows.

The current generation of numerical assessment models used by SKB employs compartment models but, at least at the time of the modelling carried out in support of Project SAFE [Lind-gren *et al.*, 2001; Karlsson *et al.*, 2001], did not link inter-compartmental transfer rates to material fluxes. Instead, the various sub-models employed direct measurements of compartmental contaminant residence times ($\sim 1/\lambda_{ii}$).

While the residence-time approach has advantages in that short-term measurements with radioactive tracers can be performed in the environment to determine a range of transfer values, the methodology suggested by equation (2) is more robust. Appendix A illustrates the potential problems with the use of residence time data. Short-term measurements will overlook long-term processes – such as those associated with solid material transport.

Basing transport on material fluxes offers the possibility of utilising a specific mass balance scheme for determining contaminant transfer. Such a foundation means that more confidence in the model is generated since the physical representation is more robust. Alternatives (residence times or transfer factors) could be used, but these are specific to radionuclides and they do not say anything about the driving forces. Neither is the translation of transfer factors from one radionuclide to other radionuclides straightforward: there must be some mechanistic understanding of the processes involved.

Understanding of the system forces is important when carrying out uncertainty (particularly probabilistic) calculations. In setting a range of residence times or transfer coefficients, it can often be the case that what appear to be reasonable variations in transfer factors or residence times imply unrealistic values or combinations of driving forces. Uncertainty calculations based on probability distribution functions of residence time and/or transfer coefficients should be approached with extreme caution.

Finally, defining transfers in terms of the contributing material fluxes helps provide a direct link to elements of the site description.

As far as transport and accumulation is concerned, the question is the extent to which elements of the SIP meet the requirements of the characterisation of fluxes in the modelled system in terms of the F_{ii} , M_{ii} , C_{ii} , G_{ii} and P_i^k .

Compartment modelling implies that there are a number of compartments in a network. The general form of transport, accumulation and exposure are written below. These help define the types of data required by assessment models. The generic nature of the expressions written here emphasises interconnectivity of the network. Simplifications are possible but these can be determined as a consequence of a review of details from the SIP. SKB [2001a] recognises the iterative nature of this process.

The inventory (in Bq) of radionuclide N in the i^{th} compartment at time t is given by:

$$\frac{dN_i}{dt} = S_i^N(t) - \lambda_N N_i + \lambda_N M_i + \sum_{j \neq i} \lambda_{ji}^N N_j - \sum_{i \neq j} \lambda_{ij}^N N_i \quad [\text{Bq a}^{-1}]$$
(3)

where the source of N into the i^{th} compartment is $S_i^N(t)$, the decay rate of N is λ_N [a⁻¹] and the amount of the precursor radionuclide, M, in i is M_i . The intercompartmental transfer rates into and out of i are defined for each radionuclide. An important purpose of the assessment model is to convert this distribution of radionuclides into estimates of radiological risk.

The concentration of *N*, as a function of time, is given by:

$$C_i^N(t) = \frac{N_i(t)}{V_i(t)} [\text{Bq m}^{-3}]$$
(4)

which accounts for the time variation in compartment volume.

Traditionally, models for long-term radiological assessments have treated geological components as dynamic entities within the model structure. Biotic components have been treated as being in equilibrium with the dynamic parts of the model. The concentration in the k^{th} biotic component of the model is then given by:

$$B_{k,i}^{N}(t) = \sum_{\substack{i=1,N_{cmp}\\p=1,N_{pth}}} K_{k,p,i}^{N}C_{i}^{N}(t) + \sum_{\substack{i=1,N_{cmp}\\l=1,N_{bio}}} I_{l,i}B_{l,i}^{N}(t) \ [\text{Bq kg}^{-1}]$$
(5)

where there are N_{pih} pathways by which the contents of compartment *i* can reach the k^{th} biotic component and there are N_{cmp} compartments in the network. The $K_{k,p}^N$ are the concentration or accumulation factors via which contaminants in *i* can accumulate in *k*. $I_{k,i}$ are intake rates of the k^{th} biotic component from compartment *i*.

Dose and risk depend on the degree of interaction between the selected groups with environmental concentrations of radionuclides given by Equations (4) and (5). For foodstuff consumption, the interaction is the annual consumption of material from a given location within the compartmental network. For airborne contaminants, the interaction is the breathing rate at a given location. For external irradiation, the exposure rate is determined by the amount of time spent at a given location. BIOMASS [2001] provides a detailed discussion of these matters and of the ways in which candidate critical groups can be identified to match the societal context of a spatially extended network of biosphere compartments.

The total dose from radionuclide *N* is:

$$D^{N}(t) = \sum_{\substack{i=1,N_{cmp}\\k=1,N_{bio}\\m=1,N_{exp}}} H^{N}_{m} E_{k,m} B^{N}_{k,i}(t) + \sum_{\substack{i=1,N_{cmp}\\m=1,N_{exp}}} H^{N}_{m} E_{i,m} C^{N}_{i}(t) [\text{Sv a}^{-1}],$$
(6)

where there are N_{exp} exposure modes² and N_{bio} biotic components in the system. The exposure rates $E_{k,m}$ and $E_{i,m}$ depend on the source material (biotic or abiotic) and the dose per unit exposure converts from exposure to dose (H_m^N) .

The total risk arising from the exposure (excluding probability of the exposure arising) is then given by:

$$R(t) = \gamma \sum_{N=1,N_{nuc}} D^{N}(t)$$
⁽⁷⁾

The summation is over all radionuclides (N_{nuc}) and uses the conversion factor identified by SSI [2001].

² Ingestion, inhalation and external exposure, as identified by BIOMASS [IAEA, 2001].

2.3 Information sources for the assessment model parameter database

Table 1 provides a summary of the main data types required by biosphere numerical assessment models. An indication of the source material and spatial scale to be used in determining parameter values is also provided.

Table 1. Sum	mary of radiologi	cal assessment	model data ty	pes. Source ma	terial indicates the
typical source	s used to provide	data for assess	ment models. A	An indication o	f the scale of appli-
cability of sou	crce data is given.	Significant loc	al-scale input	is indicated in	bold type.

Model component	odel omponent Data type		ce material	Spatial scale
Abiotic transport and	Source term and location	$S_i^N(t)$	Geosphere modelling	Local/regional scale
accumulation	Decay/ ingrowth	$\lambda_{_N}$	Radiochemical databases	Global scale
	Transfer coefficients – λ_{ij}^N	F _{ij}	Hydrology; hydrological maps [Kłos <i>et al.</i> , 1996]; catchment modelling [Nirex, 1997]	Local/regional scale
		M_{ij}	Geology; lake sediment studies [SIA, 1989]; bioturbation [Muller- Lemans and Van Dorp, 1997; IAEA, 2001a]	Local/regional scale
		C_{ij}	Ecology [e.g., Kumblad, 1999]	Local/regional scale
		G _{ii}	Gas and climatology; no	Local/ regional scale
		-9	systematic inclusion in assessment models to date	
		P_i^k	Internal characteristics of biosphere components; hydrochemistry, geochemistry and biochemistry, geology, ecology; literature review	Local scale; analogues, regional scale
Biotic accumulation	Concentration and uptake factors	$K^{\scriptscriptstyle N}_{\scriptscriptstyle k,p,i}$	Radioecological databases, literature review	Regional scale
	Intake rates	$I_{l,i}$	Animal husbandry literature, societal context.	Regional scale
Dose, exposure and risk	Exposure rates	$E_{k,m}$	Ecology, societal context, literature review; habit surveys	Regional/national scale
	Dose per unit exposure	H_m^N	International database [e.g., ICRP, 1996]	Global scale
	Risk conversion factor	γ	SSI [2001]	Global scale

Table 1 indicates that a good proportion of the numerical model database is dependent on an understanding of conditions on the local or regional scales. The process of converting the knowledge base into a parameter database can be quite involved. It is rarely possible to translate directly from site characterisation data to parameter values for use in numerical assessment models. Specific comments on the data types summarised in Table 1 follow.

2.3.1 SOURCE TERM AND LOCATION

Geosphere modelling provides the source term to the biosphere. However, it is important to recognise that the location of the geosphere-biosphere interface might change in time and space.

2.3.2 DECAY/INGROWTH

Decay constants for radionuclides are readily available from a number of sources and have global relevance.

2.3.3 SPATIAL ORGANISATION AND CONTENT

The most obviously *local* components of the model are the structural elements – the physical compartments themselves. Their extent is determined by a number of factors:

- mixing (compartmental model assumptions);
- ecosystems; and
- boundary conditions/conservatism.

The physical basis for deciding spatial extent is that within the compartment the contaminants should be well mixed on timescales that are fast compared to the timescales of processes causing transport. Commonality of internal properties is a suitable basis for deciding compartment size, but it may be necessary to sub-divide spatially extended compartments.

The ecosystems approach provides a useful and systematic method of identifying common areas. However, it is likely that, within ecosystems, there will need to be further sub-divisions as the modelling needs to account for structure from the surface layers down to the base of the quaternary deposits on the crystalline bedrock in areas where the discharge from the geosphere takes place.

A further constraint on compartment size and structure may be that the assessment requires that boundary conditions be set such that the loss of contaminants across boundaries is restricted, with the effect that radiological impacts are conservatively restricted to specified regions of the system model and thereby maximised in a controlled way.

The composition of compartments is also highly site specific but there can be a strong regional component. For example, soil type, composition and structure are likely to vary little on the regional scale. There may be wide variation in properties on short spatial scales but the dose model, taking foodstuff production from comparatively broader spatial scales, will effectively average out such variations. Detailed site investigations may not be a prime requirement in determining composition provided that a sufficient regional database is available and so long as any unique features at the local scale have been accounted for.

Not all composition information is used directly in assessment models. Knowledge of composition and chemical conditions in representative structures can be used to interpret appropriate elemental k_d -values. This approach is taken by Tits and Van Dorp [1997], where grain size of solid material is seen as the principle determinant of the strength of sorption.

2.3.4 TRANSFER COEFFICIENTS

Hydrology

It is with the determination of the transfer coefficients that the major local influence is seen: in Project SAFE the use of residence times illustrates one approach [Lindgren *et al.*, 2001]. In other programmes, there is a greater focus on water fluxes as the driving force:

- In the UK, Nirex [1997] derives water flux data from a detailed model of the catchment system which provides background data for the radiological assessment model. With this link, the radiological model is made consistent with the hydrological processes at work in the type of system under consideration. There is also the potential for the catchment model [SHETRAN-UK: Thorne, 1998] to provide input parameters to the assessment model directly.
- The approach in Switzerland [NAGRA, 1994] is different again in the way in which local information is used. Groundwater maps [see Thury *et al.*, 1994] are used to define groundwater flows. These are adopted directly as inputs to the terrestrial compartments of the *TAME* model [Kłos *et al.*, 1996]. Other water flows (precipitation, evapotranspiration, irrigation, river flows) derived from local parameters and a mass balance scheme are used to determine the fate of water in the model at run time.

Both the UK and Swiss approaches employ an explicit representation of the catchment system to determine transport resulting from water movements. Regional scale data (meteorology, hydrology) are used together with local information on the structural components of the system (area, thickness, composition, etc.) to represent local conditions.

Geology

NAGRA's approach explicitly deals with solid material transport in a mass balance framework. Again, local or regional data are used as input to the assessment model [e.g., an inferred regional erosion rate – SIA, 1989]. In the Nirex [1997] approach, solid material transport is implicitly included in the catchment modelling, which informs the choice of parameters in the radiological assessment model.

Ecology

Müller-Lemans and Van Dorp [1996] illustrate the way in which information on biotafacilitated radionuclide transport can be turned into parameters for assessment models. A detailed review is carried out to provide a small number of parameters for the assessment model (biomass activity and mass transport rate per unit area of soil).

Kumblad [1999] provides a detailed analysis of the movement of organic carbon in a particular ecosystem (a lake). In Project SAFE this is used to support the modelling of ¹⁴C transport. However, thought might be given to the inclusion of this level of detail in the transport of other key radionuclides (in parallel to water-mediated and solid material-mediated fluxes). Biotic movement would be expected to transport incorporated radionuclides in a similar way to that in which water carries dissolved species and solid material carries sorbed elements. As the focus is on *transport*, the need would be to estimate the amount of material transported from one compartment and *deposited* in another (e.g., by senescence). The work of Kumblad indicates that detailed local-scale ecological models can be constructed which could be used in assessment calculations in a way analogous to the mass balance approach in the *TAME* model for water and solid material transport.

Gas and climatology

Gas-facilitated transport has not received a great deal of attention. Nirex [1997] considers the gas pathway for the transport of ³H, ¹⁴C, and ^{220/222}Rn. The focus is on radionuclides transported in bulk gas – as gaseous material, suspended in droplets, and vapour of solid material. NA-GRA's model calculates airborne dust loads but does not include a rigorous mass balance scheme for gas in the same way as for water and solid material transport calculations. Gas transported through soils and other quaternary deposits may be accounted for in the transport of water [see, for example, Stevens, 1996].

2.3.5 BIOTIC ACCUMULATION

Radioecological databases relevant on the local scale are the primary source of information determining accumulation, concentration and uptake factors. Local conditions in the modelled area determine which of the database values are appropriate in the modelling. While it would be possible to carry out a site investigation programme to determine the uptake and accumulation factors, it is not reasonable to expect that site characterisation will be carried out at this level of detail.

Regional farming practices and other ecosystem understanding provide information for intake rates of biota. BNFL [2000] used a detailed model of bovine nutrition in determining the areas of land required for cattle farming around the Drigg site based on regional knowledge of grass yield and dietary requirements of cattle.

2.3.6 DOSE, EXPOSURE AND RISK

Dose per unit exposure factors for intake and inhalation are catalogued by ICRP [e.g., ICRP, 1996] and are globally appropriate, as is the risk conversion factor. External γ irradiation conversion factors may need to be considered on a regional basis to take into account characteristics of Swedish soils and sediments.

Model component	Stages in translation process			Biosphere model data	
Source term	Deep geology	Fracture flow model	Geosphere transport model	Release locations as a function of time and space, radionuclide flux, water flux.	
	Quaternary geology	Composition and structure			
Spatial	Hydrology			Compartment volumes, physical details,	
organisation and content	Ecology	Literature, database review		radionuclide k_ds . Species as a function of compartment location.	
	Bio-, geo-, hydro- chemistry				
	Hydrology	Sources and sinks of water	Catchment model	Water and solid material fluxes (mass balance).	
Abiotic	Geology	Sources and sinks of solid material			
accumulation	Ecology	Sources and sinks of organic carbon	Ecological model	Fluxes of organic carbon (mass balance).	
	Gas and climatology	Sources and sinks of gas	Gas transport model	Fluxes of gases.	
	Ecology	Habitat descriptions	Habitat	Accumulation and uptake factors as a	
Biotic transport and		Literature, database review		function of species mapped to spatial location.	
accumulation	Societal context	Human activities	acteristics		
	Radiological	Literature		Dose conversion factors - dose per unit exposure.	
	Galabases			Risk conversion factors.	
	Ecology	Food web		Consumption rates of specified food stuffs as a function of space.	
	Societal context	Human activities	Candidate Critical Group definition	Human consumption rates of foodstuffs as a function of location.	
Exposure,				Human occupancy factors as a function of space and activity.	
dose and risk				Human inhalation rates as a function of location and activity.	
	Radiological	Literature review		Dose conversion factors – dose per unit exposure.	
	databases			Risk conversion factors.	

Table 2. Summary of methods for deriving parameter databases for long-term radiological assessment models.

2.4 Summary of data types

Full databases for assessment models must concentrate on the areas listed below. Table 2 summarises the means by which information about the site is converted into numerical parameters in the radiological assessment modelling database.

• Spatial organisation and content

Basic identification of the types of compartments (terrestrial, aquatic, ecosystem), location and nature of geosphere-biosphere interface. Disaggregation into sub-compartmental structures (soil layers, water, sediment, etc.). Physical dimensions. Definition of the content – material structure and composition, biotic content (including societal context). Mapping to topographic map.

• Transport and accumulation (abiotic and biotic)

The driving forces for material movement – water, solid, organic carbon and gaseous fluxes across compartment boundaries – factors controlling the partitioning of contaminants between these four phases.

• Biotic concentration and uptake

Concentration factors for flora, uptake factors and consumption rates for fauna for representative species in different habitats. Identification of biota types and location – ecosystem map (linked to topographic map). Review of literature and databases, correlating structure and content to numerical ranges.

• Exposure rates and candidate critical groups

Intake rates of foodstuff from specific locations, time spent at location, inhalation rates dependent on activity and location.

• Exposure to dose and risk conversion

Radionuclide-specific conversion factors for dose per unit intake on inhalation and ingestion, external irradiation conversion factors, dose to risk conversion.

• Radionuclide/element-specific parameters

In compartment models, chemical processes within abiotic compartments are usually defined in terms of the solid-liquid distribution coefficient (k_d). Biochemical properties of radionuclides in flora are usually defined in terms of concentration factors relative to the abiotic compartments making up the habitat of the species. In fauna the amount retained in internal organs following intake (ingestion or inhalation) is generally determined by an uptake factor. These quantities are strongly influenced by local geochemical and biochemical factors in the network of compartments. Database/literature review provides numerical values which can be correlated to compartment characteristics.

With the exception of dose and risk coefficients, each of these areas has a strong dependence on local conditions, and the SIP has an important role in determining basic data. The first two areas must take into account geochemical and biochemical properties of model components since these determine element-specific behaviour of contaminants.

Other elements of the assessment process must also be taken into account. For example, the societal context of the assessment context defines the types of foodstuffs consumed by the candidate critical groups and their source. The SIP can provide the disposition of materials and resources in the region. However, additional input is likely to be required to determine the needs of models representing the site under future conditions – see Section 3.8.

The network of compartments implied by the formalism given above suggests a complex internal structure for biosphere models. Reduction towards a simplified model structure is desirable but should not pre-empt the findings of the SIP. This is recognised by SKB [2001a].

3 Correspondence of SKB SIP and PA models

3.1 Introduction

The previous section discussed the needs of radiological assessment models in terms of parameter databases and information sources. This section links the data types to the proposed SKB Site Investigation Programme (SIP) and provides comments on the suitability of the measures to be undertaken to characterise the biosphere. The material reviewed is SKB [2000] and SKB [2001a; 2001b; 2001c]

Section 3.2 reviews the relationship between the SIP and the data requirements of PA models. Sections 3.3 to 3.7 discuss the data requirements of the PA models and how specific areas of the SIP might be employed to derive the necessary data. Section 3.8 considers how model representation of future conditions might be derived. Section 3.9 provides summary comments on the suitability of the SIP as a means of defining and parameterising radiological assessment models.

3.2 SIP elements and their relation to model data requirements

The SIP is broken down into eight categories. In Figure 1 the direct correspondence of these to the areas of information required for radiological assessment models is illustrated. Biosphere PA model development is a secondary aim of the SKB Site Investigation Programme: SKB [2001a] clearly identifies the main aim of the SIP as the characterisation of the host rock in terms of its suitability for the construction of a spent fuel repository. For this reason, three major parts of the SIP play little or no role in determining data for the biosphere component of the assessment model system (thermal properties, rock mechanics, rock transport properties).

The main direct influence on radiological assessment model data from the SIP comes from the categories Surface Ecosystems, Geology, Hydrogeology and Hydrogeochemistry. Indeed, this last might, ideally, also include biochemical aspects of biota in the different habitats. The drilling programme influences the hydrological and hydrogeochemical investigations and so indirectly the characterisation of the site from the perspective of radiological assessment modelling.

3.2.1 SURFACE ECOSYSTEMS

The scope of surface ecosystems investigations is very broad in the SIP. In places these investigations are deemed to include all of the quaternary deposits - from soil to bedrock - but in much of the discussion the focus is clearly on the ecological aspects of the present-day site.



Figure 1

The correspondence between aspects of the SIP and the requirements of biosphere numerical models for long-term performance assessment.

Surface ecosystem information provides a clear basis for identifying spatial boundaries of biosphere system components. Their characteristics may be expected to vary on spatial scales of a few metres to a few hundred metres in the terrestrial environment, and even more in the marine environment. The structure and content of individual ecosystems also defines the biotic content of model compartments. Ecological information helps understand details of the food web, which, in turn, is needed to determine uptake and concentration factors as a function of model compartment. The interpretation placed on Surface Ecosystems by SKB [2001a] indicates that the societal context needed to define radiological assessment models is also considered to lie within the scope. This means that not only should the ecological aspects of the food web be considered (as types and quantities of consumption) but also the interaction of the human population with the rest of the ecosystem must be included in data assembly.

The human component of the system must be considered in terms of the interaction with the spatially distributed aspects of the PA model – food stuff sources and amounts (including material obtained from outside the potentially contaminated area), as well as occupancy of, and activities within, model compartments. A map of land use, correlated with topography, soil type and surface hydrology is the basis for a description of the nature of candidate critical groups. The linkages between SIP sub-programmes also provides basic information for estimating future land use as land rise occurs.

3.2.2 GEOLOGY

Geological investigations in the SIP influence radiological assessment models in two ways. First, the geology defines the local topography, which determines the location of habitats. Second, the distribution of fractures in the granitic host rock determines the route to the surface taken by contaminants leaving the repository. The spatial coordinates of the downstream end of the fractures define the location of geosphere-biosphere interfaces to be considered in the biosphere model – in model terms, the compartments into which the contaminants would be released. Geological processes such as soil formation and erosion also determine fluxes of solid material throughout the network of compartments.

3.2.3 HYDROGEOLOGY

The hydrological aspects of the site characterisation are of prime importance to PA model definition. This topic covers not only the deep hydrogeology of the fracture network but also the hydrology of the shallower quaternary deposits, the flows in rivers, lakes and seas, as well as the description of catchment areas and the local inputs of precipitation.

A detailed description of the catchment system provides an essential basis for determining the spatial organisation of compartments in the present-day biosphere. Radionuclide migration will primarily follow water flows so the hydrogeology strongly influences the transport and accumulation properties of the model. It also dictates the location and type of different ecosystems, and influences the location of human settlements and the kinds of human activity it is necessary to capture in the model description.

3.2.4 HYDROGEOCHEMISTRY

Hydrogeochemical characteristics influence all aspects of the radiological assessment model. The organisation and chemical composition of compartments within each ecosystem must be described in terms of the geochemistry (as well as biochemistry). These factors determine the partitioning of contaminants between water, solid, gas and biotic phases in the system as well as the uptake and concentration factors as a function of habitat. Characterisation of the hydrogeo-(bio)-chemistry allows external nuclide-specific and element-specific databases to be screened to determine parameters for PA models. Hydrogeochemistry also influences the nature and location of candidate critical groups. For example, if groundwater in aquifers is too saline, then it is unlikely that it will be exploited as a groundwater resource.

3.3 Spatial organisation and content

3.3.1 AREA TO BE CHARACTERISED

The geoscientific programme for investigation and evaluation of sites for a deep repository is set out in SKB [2000]. The basis of the SIP is defined and the focus is clearly linked to the 'site' of the repository. The 'site' includes the spatial location of the planned repository footprint and also the local environment around the site. Detailed site investigation is proposed for the local area with lower levels of detail further away from the site.

While this strategy is sensible for planning and engineering design studies, and in terms of evaluating and limiting environmental impact during the SIP and construction phases, it is not wholly consistent with the need to evaluate long-term radiological consequences. While it may be necessary to know details of the ecosystems around the repository footprint, it is of greater importance to have the details of the ecosystems around the location of potential geospherebiosphere interfaces and, further, to have correspondingly good understanding of the ecosystems 'downstream' of the geosphere-biosphere interface, where transport, accumulation and exposure will take place.

In defining radiological assessment models for long-term PA, the first element of site information to be considered is the location of the geosphere-biosphere interface. This is the point (or points) at which fractures are likely to discharge radionuclide-bearing groundwaters to quaternary deposits.

The two municipalities that have agreed to take part in the SIP are currently both coastal locations. With land rise caused by isostatic readjustment from the loads imposed during the last ice age, it is expected that sea levels will fall and that over relatively short periods the repository footprint and the current groundwater discharge points will no longer be coastal. Similar considerations applied to SKB's Project SAFE study.

This fact poses the first organisational difficulty in making use of information from the SIP. Current discharge points might be sub-seabed on the Baltic coast. Characterisation of the seabed (topography, sediment characteristics and hydrogeology) is therefore a prerequisite for characterising ecosystems and biosphere models *of the present day* when radiological impact is likely to be small and controlled. At future times, however, the geosphere-biosphere interface is likely to be lacustrine or terrestrial, but at spatial locations currently covered by the waters of the Baltic Bay. It is not possible to carry out detailed site investigations at the locations of such likely future geosphere-biosphere interfaces.

The definition of the biosphere site description models should follow from the definition of geosphere properties. However, SKB did not approach the modelling of the biosphere in Project SAFE in this way. The numerical assessment models (NAMs) used in Project SAFE give a strong impression that model components and structures were decided *a priori* and that the data requirements of the models were simplistically addressed, rather than the available site data being used to characterise model components as part of a structured process.

The important elements of the biosphere, particularly the geosphere-biosphere interface, may need to be defined primarily from a consideration of hydrogeology of the quaternary deposits. As a result of land rise, the geosphere-biosphere interface will move and the biosphere compartments receiving direct input will change with time. Some compartments become inactive as a function of time, while others may be inactive until specific events in the future evolution of the site have occurred. Still others may change their character (sea bed sediments \rightarrow lake bed sediments \rightarrow mire \rightarrow agricultural soils).

3.3.2 USE OF ANALOGUES IN CHARACTERISING GEOSPHERE-BIOSPHERE INTERFACE

Considering likely system evolution, it is important to carry out the SIP in the expectation that aspects of the system inland from the repository site may provide a subset of analogues for the future system. Furthermore, given the uncertainties in future conditions in the regional area, it is important to consider the requirement for additional non-local, non-regional analogues. Some consideration of the future evolution of the site must be included in order to make the most of local and regional information as analogues of future states. SKB appreciates this, and such considerations were included in Project SAFE.

Topographic considerations (i.e., near-surface geology) determine likely *future* catchment systems and water courses. The present-day state of surface ecosystems forms the basis for future conditions. Initial focus should therefore be on the likely kinds of geosphere-biosphere interface which are to be expected as the system evolves – terrestrial, littoral, lacustrine – plus identification of any features requiring special modelling attention.

The requirements of long-term radiological assessment models are such that characterisation of local and regional biosphere analogues could be of equal interest to characterisation of the biosphere at the present-day site location and the present-day geosphere-biosphere interface. Effort should therefore be placed on the acquisition of data from suitable local, regional, and even global analogue sites.

3.3.3 DEFINITION OF BIOSPHERE COMPARTMENTS

Identification of suitable areas and spatial volumes is important. In compartment models the primary criterion for determining the spatial extent of a compartment is that material within it should be well mixed on timescales that are short in comparison with residence times. The use of ecosystem/habitats to define compartments is reasonable since an ecosystem has, by definition, characteristic internal properties. Internal mixing by the action of biota can play an important role in validating the compartmental model approximation. Such bioturbation may also account for intercompartmental transfers. The internal structure of ecosystems/habitats is also important – relevant factors include porosity, grain size, water content, density, pH, and location of water table.

The assessment model requires a mapping of model compartments onto spatial locations in the model region. The mapping should allow for future evolution. The SIP should focus on characterising the properties of representative areas.

3.3.4 LEVEL OF DETAIL OF BIOSPHERE ASSESSMENT MODELS

The way in which 'models' will be used in representing the SIP is not clear [e.g., SKB, 2001a]. The 'models' in the SDM are, for the most part, not yet defined; neither do the assessment models yet have concrete existence. The SIP documentation refers to the use of simple and existing assessment models, meaning models with partial data coverage from existing generic or region-specific databases. These models and databases will derive from SKB's SR97 assessment of the KBS3 spent nuclear fuel disposal system [Lindgren and Lindström, 1999] and the Project SAFE assessment [Lindgren *et al.*, 2001]. However, it is likely that future assessment models for such specific well characterised sites as those considered in the SIP will be more detailed than those used in SR97 and Project SAFE because more will be known about the sites.

Kłos and Wilmot [2002] commented on the spatial organisation of the Project SAFE biosphere assessment model. The same comments apply to the SKB's biosphere modelling approach for SR97. Radiological assessment of the performance of the KBS3 disposal system may be expected to need much more spatial (and temporal, see below) organisation of biosphere concep-

tual model objects than has been the case hitherto. This additional level of detail is required because of the detailed nature of surface ecosystems. In particular, it will not be possible to say, *a priori*, where in a specific system maximum radiological consequences will arise.

3.4 Abiotic transport and accumulation

Parameters relevant to the characterisation of abiotic transport and accumulation are the fluxes of material from one compartment to another. As noted in Section 2, the model parameters correspond to water, solid material and gaseous flows. The main driving force for radionuclide transport is likely to be intercompartmental water flows, since radionuclides enter the system in solution in groundwater. However, solid material transfers can also give rise to significant contaminant transport, particularly when sorption to solid material is strong. Transport in the gaseous phase is likely to be the least important of the three physical transport modes. Nevertheless it should be considered as a means of intercompartmental (inter-habitat) transport.

The emphasis on water-mediated transport means that catchment modelling should be at the heart of site characterisation. Currently the SKB assessment modelling approach is not directly linked to catchment modelling –

turnover times are used instead. While it is possible to measure such quantities in the environment, the data collected in the SIP are more likely to characterise the fluxes themselves, and SKB is likely to develop some form of catchment-based hydrological model. This being the case, there would need to be a process by which the SIP data are converted to turnover times.

We suggest that SKB employs a more rigorous classification for biosphere characterisation, along the lines of Equation (2). A specific form for the relationship between transfer coefficients (residence times) is illustrated in Appendix A. The relationship, taken from BIOMOVS II [1996], illustrates the importance of combining FEPs for water and solid material fluxes.

Characterisation of ecosystems in terms of radionuclide residence times alone does not provide sufficient information for the representation of the system under modified (future) conditions since the relative balance between solute and solid fluxes is not known. Similarly, characterisation of the system purely on the basis of intercompartmental water fluxes is not sufficient since the important role of solid material transport would be missing.

Calculating transfers in terms of the driving forces promotes greater flexibility and transparency and provides a more direct link to environmental character. Thus, for example, the enhanced role of sediment transport in the drainage system as a result of land rise with attendant enhanced incision can be readily incorporated into the numerical model, whereas a model based on point measurements of residence times in the present day would not have the capacity to deal with changed circumstances.

Direct usage of turnover times makes implementation of mass balance less straightforward. When probabilistic calculations are undertaken to explore uncertainty, a clearer functional relationship and mass balance accounting are particularly helpful in ensuring that calculations are carried out in a self-consistent manner. Examples of this method are found in Kłos *et al.* [1996] and Kłos and Van Dorp [1999], where a water balance approach is applied to characterise intercompartmental fluxes and the corresponding transfer coefficients.

Particularly in the terrestrial biosphere, the focus of the SIP should be on the characterisation of processes driving transport, not just on a description of the system in its current state. Water flows in the drainage system are the province of the hydrogeological models in the SIP. In the terrestrial biosphere, flows in rivers and lakes are fed by precipitation, percolation and run-off. Groundwater flows are also important and there is a mixing of near-surface flows (mainly meteoric inputs to the catchment system) and deeper hydrogeological fluxes. Lacustrine environ-

ments may be modelled in a similar way to the rest of the river system, allowing for internal structures. It is important that this description has a close correspondence to the understanding of soil/sediment transport in the geological modelling. Modelling the marine system can be based on current models, with a reinterpretation of bed sediment interactions, particularly at the geosphere-biosphere interface.

The present-day system, as characterised by the SIP, then provides a 'worked example'. Water fluxes modelled on the basis of present-day parameterisation should represent, in all relevant details, the properties of the present-day system in response to present-day drivers. Confidence is then gained that changes in future characteristics (e.g., reduced precipitation in colder, drier conditions) can be adequately modelled.

Littoral and marine biospheres are more amenable to characterisation by the use of turnover times, since solid material transport is proportional to water flux. However, the origin and fate of sediment is again of relevance. Account need also be made of tidal flows – unlike the terrestrial system, flow is not necessarily in a single direction through the system of marine compartments. Ideally, flows rather than residence times should be used in the numerical model for reasons of functionality and flexibility.

SKB [2000; 2001c] do not clearly indicate that solid material transport is to be measured in the SIP. Characteristic erosion and deposition rates at soil surfaces (including material transported in run-off) is important, together with land uplift rates. Similar considerations apply to sediment transport and accumulation in river lake and marine systems. Recycling of material is an important characteristic of the geosphere-biosphere interface [Wörman, 2002]. Consideration of mass conservation in the site descriptive models would help to ensure consistency with the real world and would allow easier extrapolation to future states.

Although radionuclide transport in the gaseous phase is likely to have a limited role in the safety assessment since the amount of gaseous-phase radionuclides in groundwater is much less than the amount in solution or on solid material, intercompartmental transport of solids and solute by wind action may need to be accounted for. This can include wind erosion, deposition of dry soils, and the effect of near-surface winds on lakes and coastal waters. It is not clear which part of the SIP might deal with such matters.

A further point concerning abiotic transport and characterisation in NAMs arises from a consideration of the volume factor in Equation (8). Volumes of compartments may not remain constant, particularly in areas of net erosion, deposition, or strong uplift. The SIP needs to identify areas where such considerations might apply.

3.5 Biotic transport and accumulation

Internal mixing by biota can help define model structures. However, biota containing radionuclides can also move across model boundaries. Bioturbation by earthworms is one example often used in the past [BIOMOVS II, 1996]. However, BIOMASS ERB2B [IAEA, 2001b] also discussed the potential for contaminant transport across ecosystem/habitat boundaries as a result of the movement of biotic components. In ERB2B, account was made of detritus movement (leaf litter, etc.) leading to accumulation in low-lying regions (principally wetlands and mires). Livestock manure was also considered a valuable resource (grassland to arable land transfer) and shrubland material was assumed to be used as a source of fuel, with ash being applied to arable land as a conditioning agent.

The topics covered by the Surface Ecosystems category of the SIP will provide sufficient information to be able to characterise the assessment model. As noted in the review of Project SAFE [Kłos and Wilmot, 2002], however, there is a need to provide a clear audit trail between the characterising data and the parameter values and structures used in the assessment models. As with abiotic transport and accumulation, there is a need to map the relevant ecosystems to the topographic description.

Internal descriptions of the habitats and ecosystems must be sufficiently detailed and crosscorrelated to allow the relevant parameter values to be obtained from existing databases (e.g., soil-plant transfer factors, uptake factors for biota types). Initially a review of relevant species is required. This should be based on radiological grounds, as well as environmental protection grounds, and will identify the details of the food web to be included in the models.

SKB [2001b] describes an ecological model of carbon flows for lakes and bays, based on Kumblad [1999]. Such an approach would be of great utility as the basis for carbon transfers in assessment models. It is not clear the extent to which this approach will be carried forward in the SIP.

It is important that the ecosystem description takes into account the societal context. This means that a description of present-day society, the activities of the human population, and their interaction with and impact on the local ecology should be included in the description provided by the surface ecosystems sub-programme.

Biotic transfers must reflect natural system behaviour of the biotic component of the system as well as the patterns of behaviour enforced by the human population. This is true for the presentday system but analogue systems should also be considered – perhaps by consulting records of past human activities in the region as well as additional analogue societies elsewhere, which correspond to analogue ecosystem conditions. As the focus of the SIP is on the present-day state of the system, such matters are not well covered.

3.6 Intake and exposure

Intake and exposure determines the degree of interaction of humans with the environment. To this category belong foodstuff consumption rates (including location from which foods is obtained), the time spent at location and the corresponding breathing rate. Biotic transport and accumulation, with its characterisation of the food web, provides corresponding information for the non-human parts of the modelled system. In determining radiological exposure of the human population, it is necessary to quantify intake factors for fauna that comprise the human food chain. A land use map and ecosystem description (in terms of food web and habits and preferences of fauna) would provide details of how much foodstuff of a particular type is obtained from a particular part of the system. This information may be used to describe potential radiological impact on fauna. Concentration of radionuclides in flora can be based on soil/sediment concentrations, using the information on compartment contents discussed in Section 3.3.

3.7 CCGs – Candidate critical groups

In terms of radiological impact on the human component of the biosphere, concentrations in flora and fauna are relevant, but consideration also needs to be given to characteristic aspects of current and potential future human societies – their sources of food and the habits and preferences of consumption and other activities leading to exposure. This is the role of *candidate critical group* (CCG) modelling.

BIOMASS [IAEA, 2001b] provides detailed examples of the characterisation of CCGs in a spatially extended biosphere. In such a system it is not possible to provide an *a priori* identification of the critical group (maximally exposed group in time and space in the assessment). A range of CCGs is useful in illustrating aspects of human behaviour that characterise exposure

from a radiological assessment perspective. Radionuclide concentrations in the system, as a function of time, then identify the critical group on the basis of interactions with the environment.

To carry out such an analysis requires characterisation of human society in respect of activities and consumption habits. Within the SIP such matters lie within the scope of the surface ecosystem (i.e., humans are part of the ecosystem to be described), but it is not clear the extent to which characterisation of human activities and consumption habits are foreseen by SKB. SKB took a relatively simplistic approach for Project SAFE [Lindgren *et al.*, 2001].

The use of probabilistic techniques to simulate critical group behaviour was not recommended by BIOMASS [IAEA, 2001]. The uncertainties in defining representative behaviour by sampling from food consumption rate distribution was thought to be too complex as it would be necessary to build into the sampling combinatorial rules to avoid sample sets in which a single individual would consume unfeasibly large amounts of several types of foodstuff [see for example Kłos, 1998]. Alternatives suggested were to use local habit survey data as a representative self-selecting sample [Kessler and Kłos, 1998]. In practice, the BIOMASS approach avoids the need to use sampled data in the description of CCGs by reviewing local (and by implication analogue) behaviour in the societal context and by identifying, *a priori*, patterns of behaviour that would lead to 'central' estimates of exposure and 'higher' estimates. In addition to consumption rates, the process also includes time spent at location assuming a variety of different activities.

The BIOMASS examples indicate that higher consumption CCGs can have annual exposures between three and ten times the central value. The method may also be used to describe the potential size of such groups, so providing information on the wider radiological impact. It also provides the basis for a more informed presentation of results to members of the public.

3.8 The model system at future times

3.8.1 TRANSPARENCY IN DEVELOPMENT OF ASSESSMENT MODELS

The role of the SIP is threefold – it provides information to allow a detailed design study for a proposed repository to be carried out; it provides material to support the performance assessment component of the license application; and it allows a full environmental impact statement to be prepared with respect to the site investigation and the repository construction phase. With these aims it is not surprising that the requirements of long-term assessment models, particularly of the biosphere component, are sometimes obscured in the mass of information that will be collected in the SIP.

SKB refers to a staged development of the Site Description Model (SDM) as progressively more data become available. The data collected and the SDM will provide a detailed snapshot of the state of the site at the present day (i.e., site description at time zero: $S_D(0)$). However, the SDM is not the same as the assessment model of the site, and SKB does not provide details of how the assessment models of the site will be derived from the SDM.

It will be necessary for SKB to provide a clear audit trail from the SDM to the assessment model at time zero, as illustrated in Figure 2. This requires clear documentation of conceptual and numerical model structures. It also means that the derivation of parameter input values for numerical assessment models must follow a corresponding process as that for model development, similarly allowing a clear audit trail [cf. IAEA, 2001a].



3.8.2 TEMPORAL ORGANISATION OF BIOSPHERE ASSESSMENT MODELS

The system under future conditions (as represented by assessment model at time t, $A_N(t)$) cannot be characterised in the same way that the present-day site can. However, analogues of future states may be found and characterised in a similar way. Alternatively, the present-day model can be 'aged' by applying the influence of known external FEPs (EFEPs). The needs of this aspect of assessment modelling are not addressed in the documentation reviewed in this project. Both approaches (illustrated in Figure 3) require considerable planning and work.

In particular, there is little evidence in the reviewed documents that measurable quantities in the present-day system that can be used to define numerical components of EFEPs have been identified, although it is likely that such data will be obtained in the course of the SIP. We recommend that SKB considers what the relevant EFEP quantities might be (e.g., erosion and deposition rates, incision rates of rivers, isostatic land rise rates), and what their implications for NAMs might be.

There is an emphasis on state and boundary conditions within elements of the SIP subprogrammes. By changing initial and boundary conditions, it may be practical to determine the requirements of future NAMs on the basis of modified site description models. This is certainly true for the groundwater flow modelling (including the quaternary hydrogeology). It may also be possible in the ecosystem models to determine the flows of carbon in the system, and to represent the transfers of radionuclides in fauna moving between ecosystems, cf. movements of plant and animal products between habitats in the BIOMASS ERB2B system [IAEA, 2001b]. It would be possible to develop assessment models that track the movement of the geospherebiosphere interface as a function of time and include memory of past releases, in order to determine transfers between assessment sub-models. Such developments would be a useful complement to past SKB biosphere modelling practice.



Figure 3

Relation between assessment model at time zero and assessment model at later times. On the left-hand side, analogues are used to define assessment models of the future system state. On the right-hand side, the model of the site in an earlier state is 'aged' by the application of information on external (state-altering) FEPs.

3.9 Summary comments on the suitability of the SIP

In summary, we consider that the SKB SIP is characterising the right kind of entities within the scope of the present-day system. However, the SIP is based on a large amount of data gathering, and it appears that integration of assessment models with SIP data collection has not been a primary consideration. For the biosphere, at least, it seems that SKB has a preference to apply 'off-the-shelf' assessment models in modular format. However, in the currently available documentation there is little traceability between the SIP and assessment model requirements. Consequently, it is not easy to determine the relationship between NAM quantities and the information to be gathered in developing the SDM. It is important that assessment modelling requirements are linked to the SIP.

The timing of measurements in the SIP does not pose any real problems. The staged approach to SDM definition is reasonable and practical given the amount of work required and the detail anticipated. The limited duration of the SIP compared to the long timescales of processes at work in the biosphere presents some problems (cf. Appendix A), but the modelling approach suggested in Section 2.2 provides a means of avoiding difficulties. Future states of the systems may be approximated by considering alternative analogue sites at the present day. These analogue sites will be spatially distinct on regional scales – further inland as suggested by the eastwest succession of ecosystems noted in Project SAFE – as well as further afield.

4 Summary and conclusions

4.1 Summary of data types for assessment models

Section 2 reviews the types of data required by long-term radiological assessment models, starting with a bottom-up review of the types of modelling approach used in past assessments and which are likely to be used in the assessment of the spent fuel repository. The data types are summarised in Table 1, together with the sources of information that can be used to construct model databases. Table 2 indicates the methods by which site and other knowledge can be converted to assessment model parameter databases. The broad categories of data are:

- spatial and temporal organisation;
- transport accumulation; and
- intake and exposure.

These categories are sufficient to characterise the model in any given state of dynamic equilibrium. However, to determine suitable representative models for system states in the future, it is also necessary to assemble information on those factors affecting the system causing it to change, namely:

• system evolution and EFEPs.

4.2 Preliminary review of SKB's biosphere SIP

Based on a review of the most recent SKB radiological performance assessment [Lindgren *et al.*, 2001, reviewed by Kłos and Wilmot, 2002], there is a significant amount of work required by SKB to set up assessment models that are fit for licensing purposes:

- Information from the SIP feeds into SDMs in a well planned way. However, there is need to clarify the means by which numerical models are derived from the basic site description.
- The SDMs contain information on FEPs that are identified as relevant to the system and justified in terms of their inclusion in the conceptual model of the site. The translation of these elements into practical numerical assessment models also needs justification and description. The process of numerical model definition allows parameterisation of the site knowledge base to be addressed, taking into account the categories summarised in Section 4.1.

Assessment models in previous Swedish assessments have included most of the relevant kinds of data but the link to the site description has been weak. Carrying out a formal process of system identification, justification and description [cf. the BIOMASS reference biospheres methodology, IAEA, 2001] for the system description model and the numerical assessment model would provide the linkage required.

It is important to acknowledge that the SIP provides a detailed description of the site *under present-day conditions* and that any assessment model derived from the SDMs will be adequate only insofar as the present day reflects relevant aspects of the system at the time of potential radionuclide release to the biosphere. Future states of the system require commensurate identification, justification and description. SKB recognises that system change is a fundamentally important part of the biosphere and geosphere-biosphere interface systems, but the current SIP documentation does not give a clear picture of how data for future system configurations is to be derived or related to the SIP database. Two alternative approaches are discussed here.

Our conclusions about the SIP are as follows:

- The SIP will characterise the right kind of entities so as to allow detailed radiological assessment models to be defined. The SIP will focus on spatial locations around the repository footprint but, provided that the information gathered is treated as analogues for similar conditions at times when releases to the biosphere might occur, this is not a problem. Extending this type of information to future conditions for which there is no suitable local or regional analogue means that there is a need to identify and characterise appropriate analogue systems.
- Entities in the numerical assessment model need to be characterised in terms of the driving forces responsible for moving material around the system (and so contaminants with bulk mass flows). The internal description of model regions must also be addressed in terms of the characteristics that can lead to accumulation (e.g., sediments at the geosphere-biosphere interface). The description of the system in terms of surface ecosystems provides an excellent basis for biotic transport and accumulation modelling in the numerical model.
- The focus in SKB numerical models (in Project SAFE) is principally on turnover rates, as far as the characterisation of abiotic transport and accumulation is concerned. This approach is not sufficiently flexible to deal with the system in future states, in response to the effect of external driving forces (EFEPs). Focus on modelling abiotic transport in terms of (at least) water and solid material fluxes would help make the models more flexible. Application of the BIOMASS RBM (or something similar) would help to smooth the relation between site description and numerical model content.
- Site characterisation means that good spatial descriptions of, for example, soil types and location, ecosystems and land use will be available. The internal characteristics (soil chemistry, biotic content) will be part of this description. Radionuclide-specific parameters consistent with the internal conditions can be readily found by reference to literature and existing SKB (and external, non-SKB) databases. Allowance for the fact that internal conditions will change with time must be made. Spatially and temporally the most important varying feature is likely to be the position of the geosphere-biosphere interface as land rises. It may be necessary to include a range of interfaces with a range of properties, even for the same spatial location. Compared with previous assessments, there is a need to provide much greater spatio-temporal connectivity and to allow for flows across boundaries.

4.3 Priorities for biosphere assessment modelling

The suggested basis for radiological assessment modelling is the description of radionuclide transport and accumulation in terms of driving forces for transport – identified in Section 2 as water, solid material, organic carbon and, to a lesser degree, gaseous fluxes. By focusing on driving forces it is not only possible to build an internally consistent description of the system to be modelled as it would be in the absence of radionuclide contaminants, but it is also possible to allow for changes in external factors that influence mass transport. Such an approach is therefore useful when system evolution is to be taken into account.

To support the biosphere component of radiological impact assessments of a spent fuel repository, the emphasis should be on:

- Characterisation of the spatial extent of the modelling system. This requires that the location of the geosphere-biosphere interface be mapped onto the physical system as a function of time. Progressive refinement can be used to identify key locations in the modelled system for use in the radiological assessment calculations. Attention should be given to potential linkages and interconnections between spatial elements.
- Driving forces in the system those acting to transfer water and solid material. In catchment systems this means not only modelling groundwater flows in the quaternary sediments and precipitation, infiltration, runoff and evapotranspiration, but also the impact of geological processes such as erosion, deposition, incision and sedimentation.
- The ecosystem description should focus on the types of biota and the relevant characteristics of clearly identified ecosystems, correlated to spatial locations in the physical biosphere model. Attention should be given to potential biotic transfers in an ecologically based food web.
- Procedures for deriving radionuclide-specific parameters from a correlation of site information, literature and existing databases.
- Identification of processes characterising long-term systematic change. This should be differentiated from dynamic processes that proceed under conditions of dynamic equilibrium or near-equilibrium. The long-term forces (EFEPs) determine the rate and type of change that the biosphere system can undergo. Examples are uplift rates and medium-term and long-term modifications in climate characteristics.

The currently available documentation for the SIP indicates that most relevant site-specific data will be obtained. One area that is not well defined in the SIP is SKB's approach to the definition of critical groups in the modelled system. The societal context lies within the scope of the SIP sub-programme, Surface Ecosystems, but a clearer focus on the potential interactions of the human community with the biosphere is required.

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Appendix A

The role of solid material transport in the terrestrial biosphere

The importance of solid material as well as solute-driven transport is illustrated in Figure A-1, which shows the contribution to turnover time for soils in the BIOMOVS II [1996] Complementary Studies. The transfer rate is defined by:

$$\lambda_{ij} = \lambda_{ij}^{(solute)} + \lambda_{ij}^{(solid)} \equiv \frac{1}{\theta_i R_i V_i} F_{ij} + k_i M_{ij}$$
(A.1)

where the compartment volume is V_i , the compartmental solid-liquid distribution coefficient (k_d) is k_i , and the retardation factor is R_i , defined by:

$$R_i = 1 + \frac{1 - \varepsilon_i}{\theta_i} \rho_i k_i \tag{A.2}$$

with solid material density, ρ_i , porosity of the medium, \mathcal{E}_i , and volumetric moisture content, θ_i . The drivers of contaminant transport are F_{ij} and M_{ij} , respectively the solute and solid material fluxes.



Figure A-1: Radionuclide residence time as a function of radionuclide k_d . Soil model details from BIO-MOVS II [1996]. Contributions of solute and solid material transport are indicated, together with the combined residence time derived from

$$\tau_{ij} = \frac{\ln 2}{\lambda_{ij}} \, .$$

Significance of the shaded regions is discussed in the text.

Figure A-1 shows that at low k_d , all contaminant is in solution so that residence times are short, but increasing retardation restricts transport in solution. Below ~ 5×10⁻⁵ m³ kg⁻¹ there is no practical effect, but increasing k_d increases the residence time in solution whilst decreasing it for solid-mediated transfers. Solute transport dominates. For k_d in the range 1 to 4 m³ kg⁻¹, solid material transport has an increasing effect. For radionuclides with $k_d \ge 4$ m³ kg⁻¹, solid material transport dominates transfers. Most elements have k_d values in this crucial range [see, for example Tits and Van Dorp, 1998, for a k_d classification based on grain size and organic content]. Radionuclide solid-liquid distribution coefficients should not be included in the SIP but the factors on which they depend should. An approach similar to that used by Tits and Van Dorp [1998] can then be used to determine appropriate k_d values.

Environmental measurements of residence time (based on tracer tests) have the potential to miss the long-term component of the transport since they are temporally restricted. It is not possible to make adequate interpretation of data obtained over a few years when the relevant timescale for transport is decades or longer. The solid material component of the transport processes will therefore always by misrepresented in the observed database. Some mechanistic interpretation (cf. Equation A.1) is necessary.

Each radionuclide (dependent on sorption) would have a different residence time. The restricted timescale of the experimental work would favour low k_d or non-sorbing species. Deconvoluting observation from system response therefore contains a further layer of complexity. Estimation of the properties of solute and solid material fluxes is required.

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