A Methodology for Representing the Geosphere-Biosphere Interface in Assessment Models

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In post-closure radiological safety assessments of geological disposal facilities for radioactive wastes, models are developed and applied for transport of radionuclides through the engineered barriers and surrounding host rock towards the biosphere. Whereas the role of the engineered barriers and host rock is generally to prevent or retard the migration of radionuclides, in the more superficial strata retardation may be of less importance compared with dilution and dispersion. However, in determining the radiological impacts of possible releases of radionuclides in relation to the regulatory criteria typically employed, there is a need to evaluate the degree of dilution and dispersion in the superficial strata, together with any re-concentration that may occur. This means that appropriate conceptual and mathematical models are required to define the region between the deeper geosphere and the superficial biosphere. This region is described as the geosphere-biosphere interface and its characterization is discussed herein, based on work carried on work carried out with the BIOPROTA international collaborative forum.

I. INTRODUCTION

In the geological zone in which a repository for spent fuel or high-level waste is likely to be located, there is generally a requirement to evaluate radionuclide isolation and transport based on the present structure (possibly with limited alterations, e.g. due to seismic effects), though with changing boundary conditions reflecting large-scale changes in climate and landform (Ref. 1). Thus, the model is taken to be predictive of the future conditions of relevance at the site of interest. In contrast, the biosphere systems selected for use in the safety assessment are generally taken to be representative of the range of situations that could occur, but there is no implication that they are predictive of situations that will occur (Ref. 2).

In the superficial zone, the stability of the system is likely to be such that its particular characteristics should be taken into account in the safety assessment. Nevertheless, it will alter with time and consideration has to be given to the degree to which that evolution should be modelled explicitly and the timescale over which there should be a transition to more schematic modelling. Furthermore, the spatial scale of modelling has to be considered, as fine details of the projected distribution of radionuclides may not be needed for an overall evaluation of radiological impacts.

Models for the superficial zone (here described as the geosphere-biosphere interface or GBI) are, overall, not as well developed as those for various host rock types or for reference biospheres. Therefore, a project was undertaken within the international BIOPROTA collaboration to develop a methodology for enhancing both the conceptual and mathematical models that are available. This project has now been completed, a comprehensive, multi-step methodology has been developed, and illustrative applications of that methodology have been made to sites or regions in Scandinavia, the UK and Spain. For more details of the work described herein and a comprehensive bibliography of the relevant literature, the final report on the project should be consulted (Ref. 3).

II. OVERALL METHODOLOGY

The overall methodology is intended to be applied within the framework of a specific assessment context, with the assessment context comprising the various components set out in BIOMASS (Ref. 2), i.e. purpose, endpoints, philosophy and approach to uncertainties, repository system, site context, source term, time frames and societal assumptions.

The methodology to be applied after the assessment context has been determined is summarised in three flow charts. These are shown in Fig. 1 to 3.

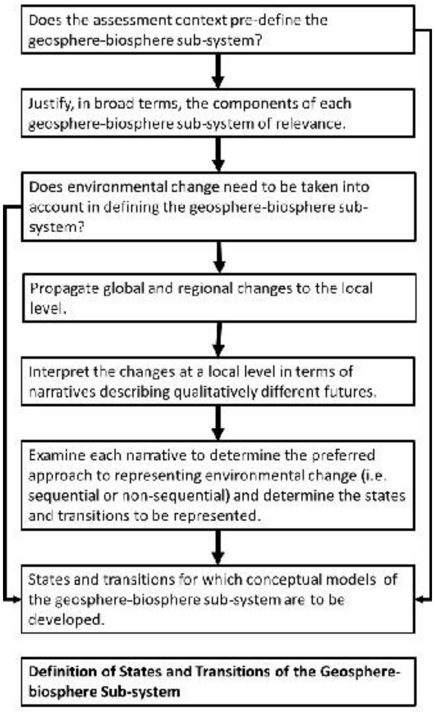

Fig. 1. Initial steps in the methodology leading to the definition of states and transitions of the GBI

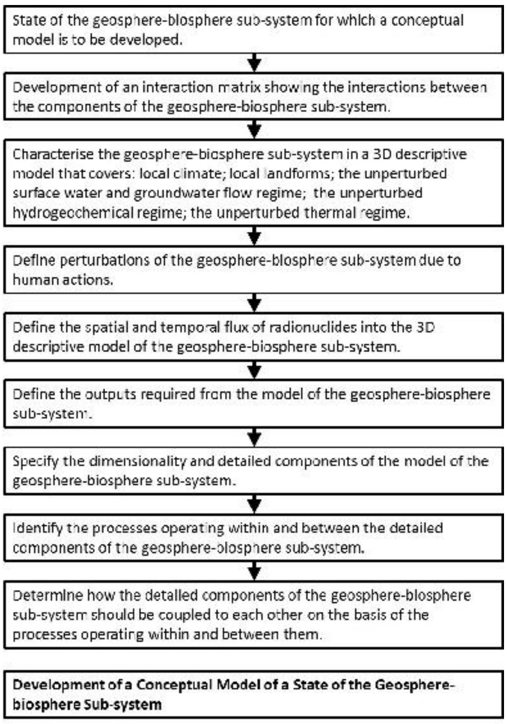

Fig. 2. Further Steps in the methodology leading to the development of a conceptual model of a state of the GBI

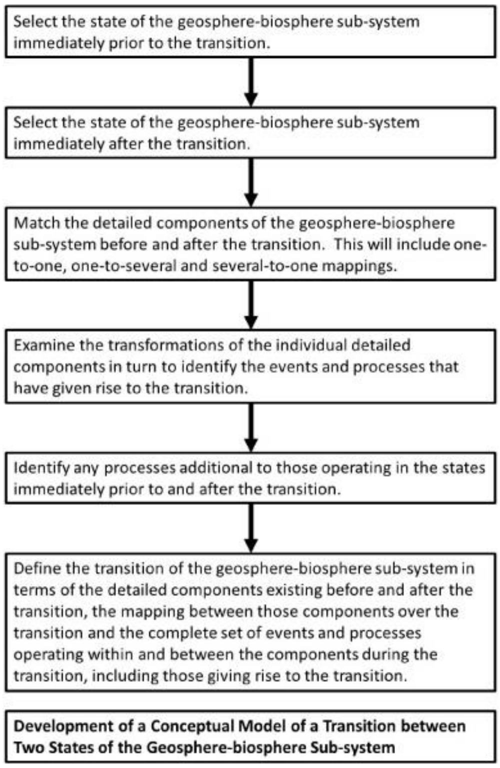

Fig. 3. Additional steps in the methodology for handling transitions between states

The methodology is broadly distinguished into three stages. In the first, sequences of states of the system and transitions between them are defined (Fig. 1). States are envisaged as time-invariant configurations of the system, whereas during transitions the dynamics of system development play a significant role in the assessment.

In the second stage, the characteristics of the individual stages are defined. This makes extensive use of interaction matrices to identify the processes that operate between the main components (features) of the system (see Section IV). In contrast to BIOMASS (Ref. 2), which emphasized the principal functional components of the biosphere, the methodology proposed here gives more emphasis to spatially defined principal components that together form a continuous 3D representation of the GBI (see Section III). This change of emphasis arises both because the GBI is more stable in time than the biosphere and because developments in mathematical modelling over the last ten years now permit a more continuous representation of the system to be adopted, i.e. the need for compartmentalization is less.

In the third stage, the characteristics of the individual states are used to provide a context for characterizing the transitions between those states. The principle adopted is similar to that described in the context of the BIOCLIM project (Ref. 4).

III. DEFINITION OF STATES OF THE GBI

In Step 1, the assessment context is reviewed to establish whether or not it pre-defines the GBI. If it does not, the components of the GBI or sub-systems to be represented are identified and justified according to an interpretation of the assessment requirements.

To a large extent, these components are similar to those for the biosphere (Ref. 1). They comprise: climate and atmosphere; geographical extent; location; topography; human community; near-surface litho-stratigraphy; water bodies; and biota.

This step precedes the consideration of environmental change (discussed below). Thus, the components of the GBI set out above can only be defined in broad terms, since they will be subject to modification as the climate and landscape alter.

If the assessment context requires environmental change to be considered, Step 2 addresses the mechanisms causing environmental change and the potential impacts of those changes through the use of External Features, Events and Processes (EFEPs) as defined in BIOMASS (Ref. 2). The overall aim of Step 2 is to provide narratives describing the various qualitatively different futures that may occur, as these narratives provide the key input to Step 3.

In Step 3, each narrative is examined to determine the preferred approach to representing environmental changes that affect the GBI. In making such a decision, account has to be taken of the narrative itself, the overall assessment context, and decisions that are being made as to how other parts of the disposal system are to be represented.

In general, a sequential approach to geosphere-biosphere representation will often be preferred. However, this leaves open the issue as to whether that representation should be continuous or discrete. In a continuous approach, radionuclide transport would be modelled through a continuously changing environment. In practice, this would imply the setting up of a set of linked differential equations representing both environmental change and radionuclide transport. In the discrete approach, radionuclide transport could be modelled as occurring within a fixed environment during each state of the GBI. However, rules would need to be provided to map the radionuclide distribution present at the end of one state to the radionuclide distribution at the beginning of the next state. Those rules would reflect two considerations: (i) the processes involved in causing the GBI to move from one state to another (e.g. transformation of a lake to a mire by terrestrialization); (ii) the model structures adopted for the two states.

Transitional regimes and transitions from one state to another (Fig. 3) will be of particular importance if radionuclides can first be accumulated in, and then acutely released from, particular environmental media. Specific processes and system elements that could lead to accumulation include: the presence of sharp gradients, such as saline fronts, changing redox conditions and the presence of organic matter; presence of hyper-accumulator plants; release to wetlands subject to rapid biological turnover and sediment accumulation. Differential effects of accumulation for successive radionuclides in a decay chain (such as that of U-238) can lead to gross departures from secular equilibrium that need to be taken into account.

At Step 4, the components of the GBI are already defined (see Step 1). For a particular stage in a narrative, these components need to be characterized in specific terms and their inter-relationships need to be identified. This can be done through the use of an interaction matrix (see Section IV).

The interaction matrix developed at this step goes beyond a listing of processes linking the various lead diagonal elements, as it briefly describes the key considerations determining the interactions, recognizes important indirect effects and notes interactions occurring at the regional scale, as appropriate.

Once the GBI has been described in terms of an interaction matrix, it can be analyzed more fully in terms of the geometrical relationships of the individual components, the spatially distributed properties of those components and the processes through which the they affect their properties, either within a component or as a consequence of interactions between components.

An interaction matrix developed as described above provides a basis for a description of the GBI that is suitable for use in developing a mathematical model. This requires consideration not only of the components of the GBI, but also their geometry, their spatially distributed properties and the processes that operate within and between them. In order to achieve this description, Step 5 of the methodology is distinguished into the following sequence of sub-steps.

- Define the local climate that will exist over the period for which the GBI is to be modelled;
- Define the local landforms that will be present over the period for which the GBI is to be

modelled. This includes their topography and lithostratigraphy, as the two are closely related.

- Characterize the unperturbed surface-water and groundwater flow regime that would apply under the specified climatic and landform characteristics.
- Characterize the unperturbed hydrogeochemical regime that would apply under the specified climatic and landform characteristics, and with the specified surface-water and groundwater flow regime.
- Characterize the unperturbed thermal regime that would apply under the specified climatic and landform characteristics, and with the specified surface-water and groundwater flow regime.
- Specify how human actions are assumed to perturb the system.
- Define the spatial and temporal pattern of radionuclide fluxes that would enter the GBI over the period for which it is to be modelled.
- Define the outputs that are required from the GBI, e.g. spatially and temporally variable radionuclide fluxes to the biosphere or concentrations in environmental media such as soils and surface-water bodies.

Once the above sub-steps, have been completed (including iterations between them to achieve self consistency, as required), it should be possible to provide a conceptual description of the GBI from which a mathematical model can be developed, or against which an existing mathematical or computational model can be audited in terms of its fitness for purpose. Having developed such a model, it will be possible to calculate the transport of fluxes of radionuclides entering the GBI in order to estimate either output fluxes to the biosphere or output concentrations in environmental media and to calculate radiation doses and other measures of radiological impact.

Where a site has been selected, characterisation of the local landforms would typically comprise a 3D visualization of the topography and lithostratigraphy either of the existing landscape or of the landscape evolved under particular assumptions. Even if a generic assessment is being undertaken, it will generally be appropriate to develop an illustrative 3D visualization of the landscape, so that a suitable abstraction of that landscape can be made for modelling purposes. It is emphasized that the visualization of the landscape in 3D is for the purposes of conceptual model development. It does not imply that the mathematical model to be derived from that visualization would necessarily be 3D. This would depend on the assessment context and the degree of homogeneity both in the landscape and in the pattern of radionuclide releases to the GBI for which the assessment was to be undertaken.

Although the GBI may not extend to the ground surface, it will generally be appropriate to define local landforms from the surface to a depth in the bedrock below the interface with the geosphere component of the system. In this way it will be ensured that the GBI is consistently embedded within the wider modelling framework.

The 3D visualization of the landscape will usually comprise a set of components, each with a well-defined geometrical extent and arranged in a space-filling arrangement, such that there are no gaps in that arrangement between the ground surface and the base of the representational domain within the lateral extent over which that representational domain is defined. Each of those components will be defined by a set of properties. Those properties will be defined in terms of parameter values or parameter value distributions at the mathematical model stage. However, for developing a conceptual model, it is sufficient to recognize the types of properties required to characterize each component.

To a large extent, the climate and topography will define the surface-water and groundwater flow domains, though account may also have to be taken of regional sources of surface water and groundwater.

In defining the groundwater flow regime, the information required is primarily the hydrological properties of the materials present in the domain and the geometrical relationships of those materials to each other. To this must be added information on the local climate, which is necessary for estimating both surface water flows and infiltration. Finally, surface water and groundwater flows across the lateral boundaries of the modelled domain need to be established.

The hydrogeochemical regime may be defined mainly by observations or by model simulations in which waters of different types are mixed in the GBI domain and react with the various types of solid that are present. Although model simulations may be undertaken at this stage, the main aim is to characterize the spatial distribution of different water types present in pore and fracture spaces in the sediments and rocks that are present in the domain.

The process of developing the hydrogeochemical model may identify aspects of the hydrological and hydrogeological model that need to be updated. Thus, there may be a degree of iteration between these sub-steps. Such iterations may also involve the acquisition and interpretation of additional data in order to resolve inconsistencies or ambiguities identified in the process of model development.

In the GBI, radioactive decay heat originating from the repository is unlikely to be significant. Therefore, the thermal regime will be largely determined by climate conditions and geothermal heat production. In broad terms, the types of thermal regime to be considered include unfrozen, seasonal ground freezing, discontinuous permafrost with taliks and continuous permafrost with taliks. Where permafrost is present, there will also be an overlying active layer subject to freeze-thaw processes.

Having defined the GBI in 3D in Step 5, it is appropriate to give consideration to the dimensionality in which it needs to be modelled and the structure of the model at the selected dimensionality.

The dimensionality of the adopted model will depend on the characteristics of the GBI and also on the assessment context. For example, if the assessment context only requires spatially averaged radionuclide concentrations in environmental media, then a lower dimensionality may be appropriate than if there is a requirement to define peak concentrations in space and the spatial extent of concentrations that are more than a particular fraction of those peak concentrations.

The dimensionality of the model can also depend on how the radionuclide flux entering the model domain is defined. For example, if the input flux is spatially distributed over a relatively homogeneous domain (such as the base of a deep agricultural soil directly overlying a bedrock aquifer that is modelled as part of the geosphere), then a 1D vertical model of the soil may be appropriate to map that flux into radionuclide concentrations at the soil surface. In contrast, if the input flux is defined without any information on its spatial extent (as with a stream tube representation of the geosphere) then a 3D model of the GBI may be required to map that input flux to a spatially distributed output flux. This might be appropriate if it was considered that most of the dispersion and dilution of the radionuclide plume occurred within the GBI.

Within the framework of the adopted dimensionality, the various components of the model need to be identified. These can be spatially distinct, e.g. topsoil and subsoil, or spatially co-extensive, e.g. rock matrix solids and pore water within the rock matrix. It is these components that provide the context for determining the importance of various processes within the GBI.

From application of the methodology described above, a 3D descriptive model of the GBI is obtained, together with an evaluation as to how that 3D model should be represented geometrically when implemented in a mathematical model. Furthermore, the key characteristics of the components of that model (e.g. porosity of the rock, chemical composition of pore and fracture waters, temperature of the rock) will have been identified. On the basis of this 3D descriptive model and its geometric representation, it is appropriate to move on to identify the processes relating those characteristics that need to be included in the model (first part of Step 7). In identifying the processes, it is helpful to characterize them under the following headings: hydrological and hydrogeological; geochemical; thermal; mechanical (e.g. erosion and deposition; freezing-induced stresses); biotic; nutrient and/or energy based.

Some indication of the types of processes of relevance will already have been obtained at the sub-system description step. However, that analysis will have been undertaken at a general descriptive level. At this later step in the methodology, the system is more precisely defined both geometrically and in terms of the spatial domains occupied by the individual components. Thus, process identification and importance evaluation can be undertaken more precisely.

In addition, if a changing GBI is being represented, it will be appropriate to take into account both natural events and human-induced perturbations.

It is emphasized that the identified processes are taken to be relevant across the whole GBI domain, though their significance will vary between different parts of that domain (for example freezing and thawing will be important in the active layer of a permafrost regime, but will not be of importance at greater depths where the sediments remain permanently frozen). Thus, process identification results in a list of processes of relevance for inclusion in the mathematical model, together with an evaluation of their significance in the various components of the GBI.

Having identified the processes and their significance, consideration can be given to their degree of coupling (second part of Step 7). The first stage is to develop an interaction matrix with the components of the GBI as diagonal elements and the processes of relevance as off-diagonal elements (see Section IV).

Note that the interaction matrix does not aim to illustrate all the processes that relate these components of the GBI. Rather, it is specifically targeted at those processes that influence radionuclide transport. Alternative matrices could be drawn up to represent other aspects of the system, e.g. heat transport. Also, the matrix can combine elements that are spatially distinct with elements that are spatially co-extensive.

In broad terms, the degree of coupling between different components of the system may be considered to range from weak to strong. The strength of the coupling, the timescale over which it operates and its directionality (i.e. whether it operates only from component A to component B or whether it also operates from component B to component A, described as unidirectional and bidirectional, respectively) determine how it should be represented in mathematical modelling.

IV. INTERACTION MATRICES

Interaction Matrices are an important tool in applying the methodology. In an interaction matrix the main components of the system under study are arranged on the principal diagonal and direct interactions between them are placed in the off-diagonal elements, using a clockwise reading convention. Interaction matrices can be used at a broad descriptive level (Ref. 3), but also at a more specific process-oriented level directed to underpinning mathematical model development. Fig. 4 shows a detailed process-based interaction matrix for a generic catchment in Lowland Britain under temperate conditions. In Fig. 4, the processes mediating the interactions are not shown. Instead they are given in a supplementary listing. Illustrative entries from that supplementary listing are shown in Table 1.

V. MATHEMATICAL MODELS

Conceptual models developed using the methodology described above can be implemented through a variety of mathematical models. At two Workshops undertaken as part of the project, mathematical models were identified and described relating to: structure, e.g. digital elevation models; landscape evolution; surface hydrology and near-surface hydrogeology; water, energy and nutrient cycling in biota and near-surface soils and sediments; hydro-geochemistry; thermal transport, e.g. of permafrost development; contaminant transport.

In addition, coupled models linking several of the above components were identified, as were models of contaminant transport in a changing landscape.

Models of climate change and of ice-sheet development are excluded from the above list. These are of considerable importance, but they require modelling at a global and/or regional scale and set a context for GBI modelling, rather than being used directly in the modelling of a specific GBI. However, they may be used to define boundary conditions used in modelling a GBI, e.g. the presence of an ice-sheet margin close to a location of interest may strongly determine the upper boundary condition for a hydrogeological model representing the GBI. Models of isostatic response and local sea level similarly condition GBI modelling, rather than being integrated into it. These models also require global and/or regional computations. Results from such models can be used locally to simulate land emergence due to isostatic uplift or to define time-dependent base levels for modelling stream incision into the landscape.

TABLE I. Examples of Interactions included in the Interaction Matrix illustrated in Fig. 4

Interactions (Numbered as in Figure 4)	**Description of the Interactions**	**Relevant Processes**
1,7; 7,1; 2,8; 8,2; 3,9; 9,3; 4,10; 10,4; 5,11; 11,5	Interactions between a solid and its included water	Sorption/desorption; precipitation/dissolution; colloid formation and dissolution; advective and dispersive transport within the solid, including diffusion into intra-particle and inter-particle pore spaces. Relevant both to the composition of the solid and its included water and to the transport of contaminants within the solid/water system.
1,14; 2,14; 3,14; 4,14; 5,14	Effects of a solid on the composition of waters formed by the mixing of meteoric and aquifer waters	Rock-water interactions that modify the chemical composition of waters with different degrees of mixing. Mainly relevant to defining the composition of waters within which contaminant transport occurs.
5,13; 13,5	Interactions between the chalk aquifer and its included groundwater outside and within the GBI that together define the aquifer end-member water that is involved in the mixing process.	Rock water interactions throughout the aquifer, taking into account the composition of the meteoric water that recharges the aquifer at outcrop. Mainly relevant to defining the composition of waters within which contaminant transport occurs.
6,7; 7,6	Exchange of water between flowing streams and soils	Recharge and discharge through the stream banks and bed. Overbank flooding and return flow. Mainly relevant to contaminant transport.
6,9; 9,6	Exchange of water between flowing streams and sand lenses where the latter outcrop in the stream bed or banks.	Recharge and discharge through the stream banks and bed. Overbank flooding and return flow. Mainly relevant to contaminant transport.

VI. CONCLUSIONS

Some general conclusions from the project are set out below. However, many, more detailed conclusions and observations are included in the final report on the study (Ref. 3) and in an associated journal paper (Ref. 5).

In the real world there is no entity that would be generally described as the GBI. Furthermore, in developing a descriptive model of a specific site there may be no need to include a distinct component relating to the GBI. Rather, discipline-specific descriptions, e.g. of the solid geology, hydrogeology, hydrogeochemistry, overburden characteristics and ecosystems, may be appropriate, with each description applicable to a spatial domain appropriate to that discipline. The role of a GBI may first emerge when the overall disposal system is being conceptualized for assessment-modelling purposes.

Although the GBI may be found useful in conceptual modelling, this may not carry over into mathematical modelling, where various tools may be employed to evaluate the significance of subsets of processes identified as being of potential significance. The conceptual model of the GBI may be used either to inform development of such mathematical modelling tools, or to audit existing tools to determine whether they adequately represent key components of the GBI and interactions between them.

In interglacial conditions, various GBIs require consideration. These divide into those associated with wells and those associated with groundwater discharge. For wells, time development of the environment is unlikely to need to be taken into account, but, for groundwater discharge, timescales of landscape development may be comparable with those over which radionuclides move through the GBI and explicit representation of landscape development may be required. This leads to the need to develop rules for mapping radionuclides from one component of the environment to another as the landscape changes.

Stochastic modelling is widely used in simplified overall assessment models. However, these are often underpinned by detailed, process-based models. The complexity of the detailed models means they are typically used in deterministic mode, with the robustness of the results obtained explored in sensitivity studies. In this study, the focus was on the development of conceptual models of the GBI and their translation into comprehensive, process-based mathematical models. These models would typically be used to inform the implementation and parameterization of simpler, assessment-level models.

A wide range of mathematical and computational tools is available for addressing issues relating to the GBI. It seems likely that most such issues could be addressed using these tools. Possibly one exception is landscape development, where existing models are primarily descriptive. However, the enhancement and application of landscape development models under changing climatic conditions is being addressed within the framework of MODARIA Working Group 6 (Ref. 1).

An important issue is the integration of the various modelling tools to address situations in which complex, non-linear feedbacks arise, e.g. the development of permafrost. In this context, there is already modelling experience available, so no fundamental issues appear to arise. A less well developed area is the integration of models of biogeochemical cycling into a wider context. Here, one of the issues is that organic materials are typically heterogeneous and poorly characterized chemically. Therefore, including organic materials directly into a general geochemical modelling tool is unlikely to be a viable option. This issue may be best approached through consideration of a limited number of radionuclides of importance in performance assessments, so that well-posed questions can be developed relating to the geochemical and biological processes controlling their transport and distribution in the GBI.

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Soils					1,6	1,7	1,8		1,10				1,14
2,1	**Boulder Clay**					2,7	2,8	2,9	2,10	2,11			2,14
		Sand lenses			3,6		3,8	3,9	3,10				3,14
4,1			**Valley infill deposits**		4,6	4,7	4,8	4,9	4,10	4,11			4,14
				Chalk bedrock			5,8		5,10	5,11		5,13	5,14
6,1		6,3	6,4		**Stream waters**	6,7		6,9	6,10				6,14
7,1	7,2		7,4		7,6	**Soil water**	7,8		7,10				7,14
8,1	8,2	8,3	8,4	8,5		8,7	**Groundwater in Boulder Clay**	8,9	8,10	8,11			8,14
	9,2	9,3	9,4		9,6		9,8	**Groundwater in Sand lenses**	9,10				9,14
10,1	10,2	10,3	10,4	10,5	10,6	10,7	10,8	10,9	**Groundwater in Valley infill deposits**	10,11			10,14
	11,2		11,4	11,5			11,8		11,10	**Chalk aquifer groundwater**		11,13	11,14
12,1			12,4		12,6	12,7			12,10		**Meteoric water**		12,14
	13,2		13,4	13,5			13,8		13,10	13,11		**Aquifer water**	13,14
14,1	14,2	14,3	14,4	14,5	14,6	14,7	14,8	14,9	14,10	14,11			**Mixed water**

Fig. 4. Interaction matrix showing principal interactions for components of the GBI for a catchment in Lowland Britain in temperate climatic conditions