The Scientific Foundations of Deep Geological Disposal
THE SCIENTIFIC FOUNDATIONS OF DEEP GEOLOGICAL DISPOSAL
This report was prepared, verified and approved for publication by Nirex under arrangements in accordance with ISO 9001.
Preface
The UK, along with other countries, has for over 50 years been grappling with the problem of what to do with high-level and intermediate-level radioactive waste. During that time there have been advances in our scientific understanding and changes in both government policy and public opinion.

From 1988 to 1997 Nirex activities were centred on research and development into one option for the long-term management of the UK’s intermediate-level radioactive wastes, namely disposal to a deep geological repository. Wide ranging scientific research was carried out to gather data, understanding and models so that the long-term radiological safety of such a repository could be assessed. For much of this period, the research included extensive site investigations, most notably around a site near Sellafield in West Cumbria. As a final stage of the investigations at Sellafield, it was proposed to construct an underground Rock Characterisation Facility there, a proposal eventually rejected in March 1997. Since then, Nirex has sought to bring the site-specific work to an orderly close and to redirect its research to give it a more generic character.

This report provides a Nirex overview of the science currently available to underpin our understanding of phased deep geological radioactive waste disposal. Whilst concentrating on our own research, we also refer to important work in this area by other organisations. We are preparing other, similar, reports that describe the engineering of a repository, waste packaging and the transport of waste packages. We hope that readers will find these reports useful. Please contact us for further information or see our website at http://www.nirex.co.uk.

Chris Murray
Managing Director, Nirex
February 2001
Executive Summary

This report summarises Nirex’s view of the scientific foundations of the deep geological disposal of radioactive wastes. It focuses upon the work that has been undertaken in support of the Nirex repository concept, that would enable a phased approach to be taken to the disposal of the United Kingdom’s intermediate-level and certain low-level radioactive wastes. ‘Phased’ in this context means maintaining the option of relatively straightforward retrieval of the wastes until society decides to close the repository.

The report is intended to provide a description of:

- the science needed to evaluate the long-term post-closure performance of the Nirex phased disposal concept;
- the relevant scientific work undertaken by Nirex and others up to early 2000;
- the status of that scientific work in terms of its addressing important issues; and
- outstanding issues that remain to be addressed in full or in part.

The report is one of a suite of reports recently produced to explain the phased disposal concept, a coherent option, in Nirex’s view, for the long-term management of the United Kingdom’s intermediate-level and certain low-level radioactive waste.

The phased disposal concept employs multiple barrier containment, making use of both engineered and natural barriers to achieve the necessary degree of long-term isolation and containment of radionuclides. Typically wastes are packaged by being immobilised in a cement matrix within a highly engineered waste container, made from stainless steel or reinforced concrete. Such wastes would be placed in disposal vaults excavated in rock at least 300 metres below the ground. The siting of the disposal facility would be on the basis that there would be a low rate of groundwater flow through the repository “host rock”, and that this low rate of groundwater flow would persist over a very long period of time. At some appropriate time after a period of monitoring, a specially formulated cement-based grout would backfill the spaces around the waste packages emplaced in the disposal vaults. Thereafter, if the society of the day decided, the vaults could be sealed and the access-ways to the repository progressively closed and sealed to specifications determined by safety considerations.

A number of technical and scientific issues – ‘outstanding issues’ - are identified to raise the level of scientific confidence associated with the phased deep disposal of radioactive wastes. These issues can be broadly separated into site-specific issues that would mostly be addressed once candidate sites had been identified and more general (i.e. non-site-specific) issues such as those relating to the performance of the engineered barriers.

The main site-specific outstanding issues relate to

- the mechanical and chemical interactions, over an extended period of time, between the excavations, the engineered barriers and the host rocks;
- the current limitations on obtaining (from surface-based investigations) representative in situ groundwater samples for reactive constituents from very low permeability rocks; and
- the effect of gas migration on groundwater movement and the localised release of radioactive gas at the surface.

The report concludes that it would be possible to obtain the requisite information over the course of a carefully structured and managed site investigation programme.
The main non-site-specific outstanding issues relate to

- the importance of palaeohydrogeological information set against its status as an emerging, semi-quantitative science;
- the limited ability of post-closure performance assessments to explicitly incorporate time-dependent processes (e.g. the effect of different flow boundary conditions) into the assessments;
- the evolution over long time scales of the engineered barriers, in particular cementitious materials such as the Nirex Reference Vault Backfill and repository seals;
- the extrapolation from laboratory conditions to in situ conditions; and
- some specific issues related to the degradation of organic materials and their ability to affect the containment of radionuclides within a repository.

The report describes work to address these outstanding issues that is ongoing within the UK national programme in the context of continued evaluation of generic disposal concepts.

More generally, some principles are identified to improve the scientific confidence in the research:

- ensuring demonstrably high quality scientific work at all times;
- the use of multiple lines of evidence, including the widespread use of natural and anthropogenic analogues (environmental features that have arisen as a result of phenomena similar to those being represented in models of the repository);
- adding value by integrating knowledge gained through traditionally segregated disciplines within science and engineering;
- adopting a clear process of model validation;
- the application of rigorous peer review; and
- peer preview (which recognises that better dialogue is required with the scientific community and, ideally, a wider range of stakeholders before a piece of scientific research is initiated).

The report deals with scientific confidence in relation to the scientific disciplines that traditionally have been involved. Such confidence is necessary but not sufficient to win the acceptance of society for a proposed solution to the long-term management of radioactive wastes. A fundamentally important principle (though not the subject of this report) is the need to look beyond the recognised experts to address issues raised by society at large. A broadening of peer preview to include general members of society will help to capture the necessary inputs. It is expected that issues raised in this way will themselves result in the initiation of new scientific work.

Taken together these principles provide guidelines to govern the development of Nirex’s future scientific research. A key challenge is to apply them and other techniques in a manner that will inspire confidence, not just in particular scientific conclusions, but in the research organisation itself.

The report concludes that, while a number of outstanding issues remain, work is in place, both nationally and internationally, to address them. In Nirex’s view none of these issues presents an overriding obstacle to phased deep disposal in principle, though we accept that not everyone agrees with this. Given the timescales anticipated to complete a review of national policy and to develop the initial strategy for any future repository development
programme, it is even possible that some of these issues will have been resolved before, if appropriate, any detailed repository proposals could be required.

A phased programme of repository development would provide many opportunities for a review of the science and associated uncertainties, and consultation with a wide range of stakeholders. Indeed, obtaining an agreed outcome from such iterative reviews of the science could be a determinant of the rate at which the programme proceeds from phase to phase.
# TABLE OF CONTENTS

**Preface** .............................................................................................................................. iii  
**Executive Summary** ........................................................................................................ iv  
1. **INTRODUCTION** ......................................................................................................... 1  
2. **THE PHASED DEEP GEOLOGICAL DISPOSAL CONCEPT** ........................................ 3  
3. **THE SCIENCE BASE REQUIRED TO EVALUATE THE LONG-TERM PERFORMANCE OF A DEEP GEOLOGICAL REPOSITORY** ....................................................... 6  
   3.1 **Scientific Information Requirements** ........................................................................ 6  
   3.2 **Underpinning knowledge base** ................................................................................ 7  
   3.3 **Iteration and integration – the scientific management process** ................................. 9  
   3.4 **Repository development and the evolution of scientific understanding** ................... 10  
4. **THE ENGINERED BARRIER SYSTEM** .................................................................. 12  
   4.1 **The role of the engineered barrier system** ............................................................... 12  
   4.2 **Containment in an engineered barrier system** ........................................................ 12  
   4.3 **The UK Inventory** .................................................................................................. 14  
   4.4 **Physical containment** ............................................................................................. 15  
   4.5 **Chemical Containment** ............................................................................................ 17  
      4.5.1 **Limitation of solubility** ...................................................................................... 17  
      4.5.2 **Redox potential** ................................................................................................ 18  
      4.5.3 **pH buffering** .................................................................................................... 18  
      4.5.4 **Sorption** ............................................................................................................ 19  
      4.5.5 **Anion exclusion** ............................................................................................... 20  
      4.5.6 **Colloids** ............................................................................................................. 20  
      4.5.7 **Degradation of organic materials** ................................................................. 22  
      4.5.8 **Alkaline disturbed zone (‘ADZ’)** ..................................................................... 22  
   4.6 **The effects of gas generation** .................................................................................. 24  
   4.7 **Criticality** ................................................................................................................ 27  
   4.8 **Summary of knowledge and capabilities** ............................................................... 27  
5. **CHARACTERISING THE GEOSPHERE** ................................................................. 29  
   5.1 **The role of the geosphere** ....................................................................................... 29  
   5.2 **Groundwater movement through the geosphere** .................................................... 31  
      5.2.1 **Understanding groundwater flow** ................................................................. 33  
      5.2.2 **Spatial variability** ............................................................................................. 35  
      5.2.3 **Fast Pathways** .................................................................................................. 37  
      5.2.4 **Excavation Disturbance** .................................................................................. 41
5.2.5 Demonstrating stable groundwater conditions ........................................................... 41
5.2.6 Time dependency ......................................................................................................... 44
5.3 Radionuclide transport mechanisms in the geosphere ..................................................... 46
  5.3.1 Sorption in the geosphere ............................................................................................ 46
  5.3.2 Rock-matrix diffusion ................................................................................................... 48
  5.3.3 Colloids ........................................................................................................................ 49
5.4 Protection of the engineered barrier system ..................................................................... 50
  5.4.1 Chemical Compatibility ............................................................................................... 50
  5.4.2 Human Intrusion .......................................................................................................... 51
  5.4.3 Natural Disruptive Events and Processes ................................................................. 51
5.5 Gas migration through the geosphere .............................................................................. 51
5.6 Site characterisation issues ............................................................................................. 54
  5.6.1 Approach to site characterisation ............................................................................... 55
  5.6.2 The effect of geological environment on site characterisation .................................... 58
  5.6.3 Going Underground: characterisation from beneath the surface ............................... 63
  5.6.4 Characterisation for repository design and construction ........................................... 66
5.7 Summary of knowledge base and capabilities .................................................................. 67
6 CHARACTERISING THE BIOSPHERE ............................................................................ 69
  6.1 The role of the biosphere................................................................................................ ..69
  6.2 The description of future biospheres ................................................................................. 69
    6.2.1 Climate and Climate Change ....................................................................................... 70
    6.2.2 Landform Change ........................................................................................................ 73
    6.2.3 Past, present & future biospheres ............................................................................... 77
  6.3 Behaviour of radionuclides in the biosphere ................................................................. 80
    6.3.1 Transport in Groundwater ........................................................................................... 81
    6.3.2 Transport as Gas ......................................................................................................... 82
    6.3.3 Radionuclide Interactions in the Biosphere ................................................................. 84
  6.4 Summary of knowledge base and capabilities .................................................................. 85
7 POST-CLOSURE PERFORMANCE ASSESSMENT METHODOLOGY ...................... 87
  7.1 Current position ............................................................................................................. 87
  7.2 Systematic treatment of uncertainty ............................................................................... 89
  7.3 Simulating time-dependent processes over long timescales ............................................ 91
  7.4 Current approach to performance assessment and model development ....................... 91
8 CONCLUSIONS .................................................................................................................. 95
  8.1 Current status of the science ........................................................................................... 95
8.1.1 Engineered Barrier System ........................................................................................................ 95
8.1.2 Geosphere .................................................................................................................................. 95
8.1.3 Biosphere ................................................................................................................................... 96
8.1.4 Performance Evaluations ........................................................................................................... 97

8.2 Outstanding Issues ........................................................................................................................ 97
8.2.1 Site-specific data ....................................................................................................................... 98
8.2.2 General issues ............................................................................................................................ 98
8.2.3 General principles ...................................................................................................................... 99

8.3 Ability to Proceed .......................................................................................................................... 99

9 REFERENCES: .................................................................................................................................... 101
List of Figures

Figure 2.1 - Multi-barrier containment ................................................................. 3
Figure 2.2 - Effect of pH on the solubility of plutonium ........................................ 4
Figure 3.1 - Structure of scientific research programme underpinning deep geological disposal .............................................................. 7
Figure 3.2 - Iterative assessment cycles ................................................................. 9
Figure 3.3 - Stepwise approach to repository development ................................. 11
Figure 4.1 - Key questions about the engineered barrier system ......................... 13
Figure 4.2 - Radioactive decay for the reference inventory .................................. 14
Figure 4.3 - Section through ILW container ......................................................... 15
Figure 4.4 - Result of underplate grouting trial using the NRVB after removal of the top plate .............................................................. 16
Figure 4.5 - pH evolution of the engineered system (schematic) ............................ 18
Figure 4.6 - Colloid size range and migration processes ..................................... 21
Figure 4.7 - Calcium carbonate formation at Maqarin (Jordan) caused by the reaction of highly alkaline groundwater with carbon dioxide in the air ........................................ 23
Figure 4.8 - (a) Gas generation rates after repository closure and (b) cumulative amounts after repository closure .................................................. 26
Figure 5.1 - Key questions about the geosphere .................................................. 30
Figure 5.2 - Schematic illustration of the groundwater, gas and human intrusion pathways .............................................................. 32
Figure 5.3 - Iterative process of groundwater flow model development ............... 34
Figure 5.4 - Downhole logs indicating the spatial variability of different properties in Borehole RCF3 at Sellafield, Cumbria .................................................. 36
Figure 5.5 - Alternative models for connectivity between clusters of flowing features (after Nirex 97) in the basement rock at Sellafield. ........................................ 38
Figure 5.6 - Illustration of a possible concept for flow through transmissive features in fractured rock (after Nirex 97) .................................................. 39
Figure 5.7 - Schematic diagram of the Äspö single fracture experiment .................. 40
Figure 5.8 - Conceptual model of faults in sandstone at Sellafield (after Nirex 97) ........ 41
Figure 5.9 - Hydrochemical conceptual model for Äspö Island showing groundwater flow and variations in chloride concentration ........................................ 44
Figure 5.10 - Europe, 18 000 years ago (from [99] based on work from the 1980s) .... 45
Figure 5.11 - Schematic influence of dispersion on radionuclide concentration .......... 46
Figure 5.12 - Radionuclide retention processes .................................................... 47
Figure 5.13 - The relationship between the programs used to assess potentially significant gas processes .............................................................. 53
Figure 5.14 – Examination of rock core removed from a deep borehole ............. 55
Figure 5.15 - General sequence of site characterisation activities................................. 57
Figure 5.16 - Mol underground research laboratory (with permission of SCK-CEN)........ 63
Figure 5.17 - Length of records for the long-term monitoring system at Sellafield......... 65
Figure 6.1 - Important questions about the biosphere .................................................... 70
Figure 6.2 - Past climate and the Louvain la Neuve climate model ................................ 72
Figure 6.3 - Limits of some identified glaciations in the British Isles (schematic).......... 75
Figure 6.4 - Past and future climate changes ................................................................. 77
Figure 6.5 - Reference biosphere developed as part of the BIOMOVS complementary studies ............................................................................................................................ 78
Figure 6.6 - Processes simulated within the SHETRAN model ...................................... 82
Figure 6.7 - Calder Hollow studies ................................................................................. 83
Figure 6.8 - Conceptualisation of soil-plant radionuclide transfer processes............... 84
Figure 6.9 - Information required to characterise the biosphere ..................................... 86
Figure 7.1 - Inputs to performance assessments ............................................................... 87
Figure 7.2 - The hierarchy of models ............................................................................... 88
Figure 7.3 - Probability density function ........................................................................ 90
Figure 7.4 - The Nirex five stage approach to model development ............................... 92
Figure 7.5 - Schematic illustration of selected FEPs on the structured FEP diagram ....... 93
1 INTRODUCTION

This report summarises Nirex’s view of the scientific foundations of the deep geological disposal of radioactive wastes. It focuses upon the work that has been undertaken in support of the Nirex repository concept, designed to enable a phased approach to be taken for the disposal of the United Kingdom’s intermediate-level and certain low-level radioactive wastes.

The report is intended to provide a description of:

- the science needed to evaluate the long-term post-closure performance of the Nirex phased disposal concept;
- the relevant scientific work undertaken by Nirex and others up to early 2000;
- the status of that scientific work in terms of its addressing important issues; and
- outstanding issues that remain to be addressed in full or in part.

The report is one of a suite of reports recently produced by Nirex to explain the phased disposal concept. A high level description of waste packaging, waste transport, repository design and operation (including the option for long-term monitoring and retrieval), and safety is given in [1]. Nirex believes that this demonstrates that a coherent concept exists as one option for the long-term protection of human health and the environment from the radioactivity in the intermediate-level and low-level wastes under consideration. The specification and design of the generic repository concept and associated transport system, and assessments of the safety of the transport system, the operation of the repository and of a closed repository are given in more detail in a set of six “generic documents” [2, 3, 4, 5, 6, 7]. These generic documents are intended to translate the current understanding of scientific and technical issues into the coherent concept for waste management.

The Generic Performance Assessment [7] translates the understanding of the science, which will be described in this report, into an evaluation of the long-term safety and environmental protection that would be afforded by the concept. The methods and approaches used in the evaluation of long-term safety and the physical and chemical processes important to the long-term safety of a closed repository are described in an associated report [8].

In this report we identify outstanding scientific issues that remain to be addressed in full or in part. While we believe the resulting list of outstanding issues is comprehensive, we recognise that others may take a different view (e.g. [9, 10]). We expect that consultation with the public (through a broadening of the peer preview process for instance) will extend this list, though we have not attempted to anticipate these developments here. The company’s proposals for addressing the outstanding issues identified here will be described in another report [11], specifically designed to seek feedback so that outside influence can be brought to bear on the programme and other outstanding issues can begin to be identified and addressed.

The report “Nirex 97” [12] and its summary [13] show how an extensive set of field data was integrated into a site-specific assessment of the post-closure performance of a repository at Sellafield. This integration is viewed as a crucial element in the evaluation of long-term safety [14]. Nirex is currently not involved in a search for a site for a phased disposal facility, and is concentrating on continued evaluations of the generic concept. However, it is necessary to assess the adequacy of current capabilities in characterising sites and integrating the information obtained into performance assessments, so reference will be made in this report to the Company’s past work at Sellafield.
It is widely recognised that the development of a long-term safety case for a deep geological repository is best conducted as a stepwise process, where confidence is evaluated and demonstrated incrementally to support each successive decision towards the licensing and authorisation of operation of the repository [15]. A comprehensive understanding of all scientific issues is not even achievable at the early stages of development in the absence of site-specific information, and more generally the status of information and understanding required would be expected to increase with successive stages in the programme.

In accordance with current policy on radioactive waste management [16] and regulatory guidance [17], the report deals with the science of deep geological disposal of those wastes that have in the past been in the Company’s remit. It is recognised that the House of Lords’ Select Committee on Science and Technology called for an integrated strategy on waste management [18] such that the management of high-level waste and other materials that might be declared wastes, such as uranium, plutonium and spent nuclear fuel might require to be considered along with the intermediate-level and low-level wastes covered explicitly in this report. Particularly given the appreciable amount of long-lived actinide elements and fission products that are present in much of the intermediate-level waste, the requirements and scientific principles of the same long-term management of these materials would be expected to be very similar. Therefore, much of the content of this report is expected to be equally applicable to the possible deep geological disposal of these other materials, particularly in respect of the behaviour of radionuclides in the geosphere and biosphere. It is hoped that the report will provide some of the necessary information to judge whether phased geological disposal is a viable option and whether sufficient information exists that, were the option to be taken forward, the necessary design and site selection processes could be initiated with sufficient understanding of the relevant issues.

The scientific principles of the Nirex repository concept are outlined in Section 2 and the science base required to support the evaluation of its long-term safety is described in Section 3. The current understanding of each of the three main components of the overall disposal system, viz: the near field\(^1\); the geosphere\(^1\) and the biosphere\(^1\) is presented in Sections 4, 5 and 6 respectively and the current status of performance assessment methods is given in Section 7. Section 8 presents the conclusions of the report. There is an extensive listing of references used in the report to give readers access to the more detailed information that supports the synthesis presented here.

\(^1\) The repository system is conventionally divided into three components, the near field, the geosphere and the biosphere. For the purposes of this report, the near field is defined as the excavated volume of a repository containing the waste packages and the backfilling and sealing materials; the near field also includes the chemically disturbed adjacent host rocks. The geosphere is defined as all the rocks surrounding a repository while the biosphere includes the atmosphere and the Earth’s surface, including the soil, surface water bodies, seas and sediments. While such divisions are convenient, it needs to recognised that there will be significant overlaps between neighbouring components.
2 THE PHASED DEEP GEOLOGICAL DISPOSAL CONCEPT

In common with the approach adopted in many other national programmes, and endorsed by international organisations, Nirex has developed a concept [1] of multiple barrier containment designed to ensure the long-term safety of a closed repository containing the nation’s ILW and certain LLW (Figure 2.1). The multiple barrier containment concept makes use of engineered barriers (both physical and chemical) and natural barriers, working in conjunction with one another to achieve the necessary degree of long-term isolation and containment of radionuclides by preventing or limiting their movement from the repository to the human environment.

Figure 2.1 - Multi-barrier containment

Typically, wastes are packaged by being immobilised in cement within a highly engineered waste container, made from stainless steel or reinforced concrete. Such wastes would be placed in disposal vaults excavated in rock at least 300 metres below the ground. The siting of the disposal facility would be on the basis that there would be a low rate of groundwater flow through the repository “host rock”, that there would be a sufficiently long time for any radioactive materials in the groundwater to travel from the disposal vaults to the human environment at the surface and that there would be appropriate levels of reduction and dilution of dissolved concentrations of radionuclides along the travel path. In addition, the groundwater chemistry would be relatively benign towards the engineered materials in the repository so as not to be detrimental to their required safety functions. The role of the geosphere is described in more detail in Section 3.1.

At some appropriate time after a period of monitoring, if the society of the day so decided, a specially formulated cement-based grout could backfill the spaces around the waste packages emplaced in the disposal vaults. Thereafter, again at periods to be determined by the society of the day, the vaults could be sealed and the access-ways to the repository progressively closed and sealed to specifications determined by safety considerations.
The cement-based backfill to be placed around the waste packages represents an important engineered barrier within the overall concept. Its principal purpose is to provide chemical conditioning of groundwater that would inevitably come into the disposal vaults and eventually come into contract with radionuclides in the wastes. The backfill is designed to ensure that the groundwater would be maintained in an alkaline condition (“high pH”) for very long periods of time (at least one million years). This is because the solubility in water of a number of radionuclides such as plutonium – 239 or uranium – 238 that are potentially significant for long-term safety is very low under alkaline conditions. Figure 2.2 shows how the solubility of plutonium varies with the pH of water.

The use of cement-based backfill as an important barrier in the Nirex repository concept was determined after considering a range of options. Its selection was based not just upon the benefits of controlling radionuclide solubilities at low levels, but also because, if suitably specified, its safety-relevant properties could be relied upon throughout the engineered near-field of the repository and for the extended period of time required. In particular, by providing a homogeneous chemical-buffering of the water chemistry at an alkaline pH the solution chemistry of most radionuclides is made simple and predictable, compared with a situation where the chemistry would depend upon the interaction of inflowing groundwater and the various materials present in waste packages in the repository. The concept relies upon the inevitable dissolution by groundwater of materials in the repository: the evolution of the repository contents towards equilibrium with its natural setting thus provides a continuing means of containing radionuclides rather than being detrimental, as would be the case for degradation of a physical barrier.

**Figure 2.2 - Effect of pH on the solubility of plutonium**

![Graph showing the effect of pH on the solubility of plutonium](image-url)
This ‘cementitious repository’ concept, based on chemical containment, is common to the approach taken by many waste disposal agencies (e.g. [19], [20]) needing to find solutions for the long-term containment of intermediate-level (as opposed to high-level) waste. A cementitious concept also has the advantage of ensuring compatibility with the wasteforms, which predominantly entail cement encapsulation of the waste. The Nirex Reference Vault Backfill (NRVB) has been designed to afford other contributions to the isolation and containment of radionuclides, over and above the uniform, long-term control of the solubilities of actinides and other metallic elements. These are described in [21] and are discussed in Section 4.
3 THE SCIENCE BASE REQUIRED TO EVALUATE THE LONG-TERM PERFORMANCE OF A DEEP GEOLOGICAL REPOSITORY.

Section 2 describes the principles of multiple barrier containment and their application within the Nirex repository concept. In this section, the scientific information required to evaluate the long-term performance of a repository is outlined.

3.1 Scientific Information Requirements

Science and engineering are required to underpin development of design concepts for the particular wastes identified for disposal and to evaluate how the repository system will behave. The design and behaviour of the repository will determine the levels of safety. Safety associated with the transportation of waste packages, the management and operation of the repository and the potential long-term environmental impacts following repository closure all contribute to the viability of the proposed development. However, scientific research and development is particularly relevant to the assessment of long-term post-closure radiological safety because of the need to:

- understand the physical and chemical behaviour of the combination of materials contained within the repository (noting that, following repository closure, there is potential for the materials to evolve and mix, modifying the physical and chemical environment within the repository);

- identify how the materials and conditions within the repository could affect the surrounding natural environment;

- identify the potential for radionuclides entrained in groundwater or gas to leave the engineered repository and reach the accessible environment, and the associated pathways and kinetics for this transport; and

- consider the behaviour of the repository contents and surroundings over very long timescales.

From this flows a need to develop models of the repository and its surroundings in order to evaluate the future performance of a repository. Central to model development is validation. This is a procedure in which a model is used to make predictions that can then be tested against observations [e.g. [22]]. It is important to note, however, that validation is rarely a ‘one-off’ event; more usually it is an intermittent process whereby a model may be tested, evaluated and improved or replaced. The ultimate aim of validation is to demonstrate that a model is ‘fit for purpose’. The adoption of well-defined validation procedures and protocols helps to show that the validation has been carried out objectively and appropriately.

A broad-based scientific research programme is required. This programme needs to build an understanding of the repository system (the repository itself and its surrounding environment) and how it will perform over time. The research needs to investigate the processes and features that determine radionuclide behaviour in each of the main components of the overall system, viz: the engineered barriers, the geosphere and the biosphere. Research is also required to develop methods to integrate this information in evaluations of radiological risk and environmental impact. (Figure 3.1).
Information results from a range of pure and applied research studies and is used to support a wide range of activities aimed at developing and building confidence in repository development proposals. The level of scientific information considered sufficient to support these activities varies, both from activity to activity, and at different stages in the development of repository proposals. The levels of scientific information required to support different stages of a repository development programme are discussed below. In general terms, scientific information relating to the long-term post-closure behaviour of a repository is used to:

- develop and adapt realistic disposal concepts and engineering designs and identify suitable locations for a repository;
- identify the range of issues that need to be addressed when modelling the future evolution of the proposed repository under site-specific conditions;
- synthesise the wide range of information into a form suitable for use in modelling;
- provide the scientific basis on which the judgement of recognised experts can be used to augment imperfect knowledge about the behaviour of the repository system; and
- satisfy a wide range of technical and non-technical stakeholders that repository proposals are firmly based on the application of good science and best practicable means to ensure risks are as low as reasonably achievable.

The first four items focus on the process of understanding and evaluating the potential performance of the facility once it has been closed (post-closure), and is no longer under active human control (see section 3.2). The last item identifies the importance of widespread consultation and scientific debate to establish whether confidence can be built in the disposal concept, in the organisation proposing repository development and in the understanding of risks from a proposed repository (see section 3.3).

### 3.2 Underpinning knowledge base

Research into the engineered barrier system needs to establish the inventory of materials to be placed within the repository or used in its construction, and then to consider how it will...
evolve once human control has been removed. Generic and site-specific research into the post-closure performance of the waste packages and other engineered barriers provides the basis for determining the effectiveness of the engineered barrier system in containing radionuclides in the future. Key issues are as follows.

- The length of time for which the engineered barriers would physically contain radionuclides.
- The length of time for which the engineered barriers would chemically contain the radionuclides; the amounts of radionuclides (which ones and at what concentrations) that would be present in groundwater within the repository at different times. These radionuclides would be available for migration to the surface via the groundwater pathway.
- The rate at which gas would be generated within the repository and the amounts of radionuclides that the gas would contain. These radionuclides would be available for migration to the surface via the gas pathway.

Research into the geosphere needs to explore the mechanisms by which radionuclides can be transported through the geosphere. This is governed by the many physical and chemical interactions that can occur between the rocks, groundwater and gas in the geosphere. Key issues are:

- the amount of groundwater moving through the repository and its surrounding environment, its rate of movement and the pathways taken through the geosphere;
- the transport processes that operate on solutes entrained in groundwater migrating through the geosphere;
- the level of protection to the engineered barrier system provided by the geosphere. This involves protection against chemical degradation as well as protection against natural and anthropogenic disruptive events;
- the rate at which radionuclides entrained in gas can move through the geosphere back to the surface; and
- the ability to characterise the geosphere at a particular repository location.

Knowledge about the biosphere needs to consider the range of possible biosphere conditions that could occur over millions of years into the future. Biosphere research therefore focuses on the general issues and processes that control biosphere evolution and change. Key issues are:

- the range of possible biosphere conditions into which radionuclides from the repository could be discharged over the timescale of interest; and
- the behaviour of radionuclides once discharged into a biosphere having those characteristics.

It is also very important to understand the coupling both between important processes and between the different components of the repository system. For example, groundwater movement in the geosphere could be modified by the presence of gas (and vice versa), climate change could result in altered geosphere conditions as well as biosphere conditions, the construction of engineered barriers could affect the properties of the immediately surrounding geosphere and all these processes are likely to vary (at different rates) over the very long timescales under consideration. Integration between different aspects of the scientific and engineering programme is therefore very important.
3.3 Iteration and integration – the scientific management process

Performance assessments enable evaluation of overall system behaviour and of its component parts, of sensitive aspects of this behaviour, of the approach to compliance with safety-based regulations and facilitate the design and optimisation of the system as increasing amounts of engineering and site-specific data flow into the project. It is during a performance assessment that much of the scientific information is drawn together and integrated into a representation of the whole repository system.

Performance assessments are used throughout the course of a repository development programme [8]. At any point in the programme, they can be used to represent the state of knowledge about the future behaviour of the repository and identify areas of uncertainty. Further scientific research can then be undertaken to reduce uncertainty and build confidence by testing whether the performance assessment models are appropriate.

Figure 3.2 - Iterative assessment cycles
Iterations between performance assessments and the design and research work on which they are based enables the overall understanding of the system to be progressively developed. Therefore, in practice, performance assessments for a particular repository concept are likely to be undertaken over a number of years in an iterative series of “assessment cycles” (Figure 3.2). Each assessment will build on the previous one, perhaps by the use of improved data or refined models. The performance assessment is therefore inextricably linked to ongoing scientific research regarding the behaviour of the engineered barrier system, the geosphere and the biosphere.

Once site investigations are underway the integration of site data becomes an important input to the iterative process. Much has been learned from the iterative process developed by Nirex in its investigations at Sellafield. Starting in 1989 Nirex undertook a programme of site characterisation consisting of an integrated programme of geological, hydrogeological, geochemical and geotechnical studies at Sellafield. The process of characterisation involved iterating between data gathering, interpretation and groundwater flow modelling. Each iteration provided an evolved understanding of the area, which had the potential to be used in site evaluations [23]. A preliminary assessment of the groundwater flow pathway at Sellafield “Nirex 95” [24] was based on the geological, hydrogeological and geochemical understanding presented in Nirex Report 524 [25] and arising from additional investigations and studies carried out up to mid 1994. “Nirex 97” [12] was based on a revised understanding, reported in a series of topical Nirex reports and summarised in Nirex Report S/97/008 [26].

3.4 Repository development and the evolution of scientific understanding

A repository development programme would be carried out in a progressive, phased manner. Each phase would be designed to meet a specific milestone within a waste management policy and should involve a programme of public consultation.

Figure 3.3 illustrates such a stepwise process of repository development. At the outset there would be a significant amount of conceptual work to establish consensus on matters such as waste inventory, engineering concept, retrievability options and approaches to selecting and developing a site. Following this, the next main phase is the siting process, to determine whether a site could be found that was suitable for the development of a repository. The third phase would be the construction and commissioning of the repository and the fourth phase would be the operational stage of continual waste emplacement. This could be followed by a discrete stage of underground storage and monitoring (maintaining the option of relatively straightforward retrieval of the wastes), followed at an appropriate time by a final stage of decommissioning and repository closure if the society of the day so decided. Each of these stages, even the last, can be reversed, albeit with increasing difficulty and investment of resources at each successive stage.

It is not necessary to have met all scientific information requirements at the first stage (the conceptual stage) in a repository development process. An overall understanding of the repository system can be developed progressively. However, information from generic research programmes is required. This information is used to develop initial hypotheses regarding repository performance based on initial design concepts. It is also required to build confidence that appropriate methods are available to obtain the necessary scientific information for later stages in the repository development programme. Together, these elements of the conceptual phase establish the viability of taking the concept forward.
Figure 3.3 - Stepwise approach to repository development
4 THE ENGINEERED BARRIER SYSTEM
This Section summarises research into the engineered barrier system, primarily focussing on the cementitious engineered barriers adopted for the Nirex disposal concept for low and intermediate level wastes.

4.1 The role of the engineered barrier system
Depending upon waste type, the ‘engineered barriers’ would normally consist of
- a solid wasteform;
- a metal container and/or ‘overpack’; and
- a backfill (‘buffer’ in some concepts).

These engineered barriers form an important part of the near field, defined on page 2. The role of this engineered barrier system in the safe isolation of wastes varies according to concept, waste type and geological environment, but in most concepts, the engineered barrier system is envisaged as the initial barrier to the mobilisation and migration of radionuclides. In general, an engineered barrier system is designed to contain radionuclides sufficiently so that short-lived radionuclides have been removed from the repository system by radioactive decay, and the concentration of most long-lived radionuclides has been reduced to insignificant levels.

The Nirex disposal concept follows similar principles. Typically, physical containment is provided by mixing the waste with a cement encapsulant within a specially designed container (e.g. a 500 litre stainless steel drum). The chemical conditions in the engineered barrier system are dominated by the presence of large amounts of Nirex Reference Vault Backfill (NRVB), a cement-based material [21]. The resulting high pH conditions, together with the limited availability of oxygen, will act to hinder corrosion of the waste containers.

After the passage of hundreds, possibly thousands, of years, some of the content of longer-lived radionuclides may have escaped from the waste containers either as gas (see Section 4.6) or in solution in the surrounding repository water (the ‘near-field pore water’). The high pH conditions that result from the presence of the NRVB will reduce the solubility of many of these radionuclides in the near-field pore water to very low levels; in addition, many of the radionuclides will be sorbed onto the NRVB. This containment of radionuclides by solubility reduction and sorption is often called chemical containment. The products of the corrosion of the waste packages, and the waste encapsulation materials, may also sorb radionuclides. Physical and chemical containment, combined with a very low groundwater flow rate, are intended to ensure that any release of radionuclides from the near field to the geosphere (the rocks surrounding a repository) would occur extremely slowly.

Figure 4.1 reproduces the key questions about the engineered barrier system raised in Section 3 and identifies the most significant factors that affect them. The state of knowledge about these important factors is summarised in the following discussion and is discussed in more detail in the underlying references.

4.2 Containment in an engineered barrier system
In general, containment in any engineered barrier system will depend on the nature of the wastes, the way in which they are packaged, the design of the repository and the other materials used within the repository environment. The engineered barriers need to be
designed so that they are compatible with each other. Interactions between different materials will affect the amount of physical containment afforded by different barriers.

**Figure 4.1 - Key questions about the engineered barrier system**

<table>
<thead>
<tr>
<th>RESEARCH TOPIC</th>
<th>KEY QUESTIONS</th>
<th>AFFECTED BY</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evolution of the engineered barriers over time</td>
<td>How long will radionuclides be contained in the repository?</td>
<td>Repository design</td>
</tr>
<tr>
<td></td>
<td>What amount of radionuclides will dissolve in groundwater?</td>
<td>Inventory</td>
</tr>
<tr>
<td></td>
<td>What amount of radionuclides will be entrained in gas emitted from the repository?</td>
<td>Physical barriers</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Solubility</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Redox potential</td>
</tr>
<tr>
<td></td>
<td></td>
<td>pH</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sorption</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Colloids</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Organic material</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Interactions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Gas generation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Inventory</td>
</tr>
</tbody>
</table>

In addition to containment of the emplaced wastes in cells or vaults, closure of a repository will entail the backfilling and sealing of the repository access-ways (shafts, roadways etc.). This is likely to be achieved through a combination of mass backfill material (perhaps previously excavated rock, possibly mixed with bentonite or cement) and specially engineered seals. Through use of appropriate backfill material and careful seal placement, the broad aim would be to produce an effective permeability for the filled-in openings that is at least as low as that of the surrounding rocks. Parts of the seal/backfill system may also be required to withstand high hydraulic head gradients during the resaturation period but, once resaturation was complete, the hydraulic head gradients would be low. Given the timescales over which the seal/backfill system is required to function effectively, an important issue here is the longevity of the engineered seal/backfill system. This largely devolves into a site-specific question regarding the chemical and physical interactions between the seal/backfill system and the surrounding host rocks and groundwaters. For those parts of the seal/backfill system positioned close to repository, interactions with the various components of the near field (waste leachate, buffer, vault backfill etc) would also need to be considered.

While backfilling and the construction of seals is common practice in mining, the long time scales appropriate to radioactive waste disposal increases the difficulty of the task and suggests that a significant amount of careful work will be necessary to demonstrate the adequacy of the adopted seal/backfill system.
A Nirex repository would be specifically designed to contain the wide range of intermediate level wastes that are produced in the UK. In the Nirex repository concept, the long-term containment of long-lived radionuclides in the near field primarily relies on chemical containment through the creation of a cementitious repository environment, brought about by the emplacement of NRVB around the waste packages. This environment also promotes the physical containment of the wastes both by reducing container corrosion and by providing an environment that is compatible with the encapsulated wastes, most of which employ cement grout as an encapsulant. The use of a relatively permeable vault backfill (the NRVB) also allows the escape of gas from the repository, preventing any unacceptable build up of pressure from gas produced by corrosion and other processes.

4.3 The UK Inventory

Nirex and the Department of the Environment, Transport and the Regions maintain and publish a national inventory [27] of existing wastes and forecast future waste arisings. The inventory contains a range of radionuclides with a wide range of half-lives (which is the time it takes for radioactivity to decay by 50%). They include significant quantities of long-lived radionuclides such as chlorine-36, iodine-129, plutonium and uranium isotopes and their radioactive ‘daughter’ radionuclides.

Figure 4.2 shows how the radioactivity of a “reference inventory” [27] of radionuclides would decay over time and illustrates that the majority of radioactivity would decay over the first few thousands of years. Only a few radionuclides would remain radioactive over very long timescales.

Figure 4.2 - Radioactive decay for the reference inventory

Operations at nuclear facilities give rise to wastes in a variety of physical and chemical forms [27]. For example, slurry type waste is generated by the use of ion exchange chemicals to clean up liquid effluents from reactor operations and the reprocessing of spent nuclear fuel. Other waste forms include metallic fuel cladding, and plutonium contaminated materials such as plastics and filters that are generated as part of reprocessing.
nuclear plant is taken out of service or decommissioned, large items of metallic components and concrete rubble wastes are generated which may be contaminated with radionuclides and therefore require treatment as wastes.

The waste contains a range of materials including metals and organic materials whose long-term degradation can impact on the design of the repository concept and its performance. Organic materials in the waste can, for example, degrade to produce a range of complex organic molecules that have the potential to influence the solubility of some radionuclides in the waste. For this reason it is necessary for the inventory to include data on the non-radioactive materials in the waste.

4.4 Physical containment

The waste packages provide the first barriers to radionuclide migration (Figure 4.3). The long-term behaviour of the waste packages has been the subject of extensive research by Nirex and by the waste producers for many years [28]. Waste evolution and package performance will vary depending on different materials content and package designs. For a 316 stainless steel container, the time required for penetration by corrosion under the anaerobic conditions appropriate to the post-closure period is of the order of 10,000 years [29]. However, most metal containers are likely to be vented to allow gases to escape. These vents will allow the release of dissolved radionuclides once the waste packages have become resaturated. The waste encapsulation grouts are also expected to provide an important physical barrier to radionuclide release from the waste packages. Pristine waste encapsulation materials are expected to have a low permeability and diffusivity relative to that of the NRVB [30], and will limit radionuclide release. In particular, groundwater flow will be largely excluded from low-permeability waste packages, and instead channelled through the higher permeability NRVB around the waste packages. In such circumstances, the release of radionuclides will be limited by the rate of diffusion of radionuclides from the waste packages to the backfill. Computer programs, such as RARECAN [31] have been developed by Nirex to describe the impact of container perforation on radionuclide release.

*Figure 4.3 - Section through ILW container*
The encapsulating grout in a waste package will not remain in pristine condition in the long term. In particular, corrosion of metal wastes will lead to a volume expansion, and cracking of the grout may ensue (as well as possible rupturing of the waste containers). Cracking of the grout will increase its permeability and diffusivity, and result in an enhanced release of radionuclides compared to the behaviour of the pristine material. The computer program NAMMU [32] has also been used to examine the impact of container design on radionuclide release. Calculations suggest that, for certain vent designs, highly soluble and poorly sorbing radionuclides can be released from containers over timescales in the order of a few hundred years. It could then take many thousands of years for these radionuclides to travel through the geosphere to reach the surface.

The NRVB (Figure 4.4) is designed to be relatively porous and permeable. This facilitates the development of uniform chemical conditions and uniform radionuclide concentrations within repository vaults. It also enables gases to migrate readily out of the near field, preventing an unacceptable pressure rise.

*Figure 4.4 - Result of underplate grouting trial using the NRVB after removal of the top plate*
4.5 Chemical Containment

In the Nirex repository concept, two processes contribute to chemical containment:

- limitation of solubility; and
- sorption.

These processes depend on, or are affected by, a number of other factors, notably redox potential, pH, anion exclusion, colloid production and the degradation of organic materials. A consequence of the cementitious repository environment is the chemical disturbance of the repository host rocks leading to the formation of an alkali disturbed zone (ADZ). All these aspects are discussed in this sub-section.

4.5.1 Limitation of solubility

A few radionuclides (e.g. chlorine-36) have sufficiently high solubility and/or are present in the repository in sufficiently low quantities that they may be assumed to exist only as solutes in the near-field pore fluid. (The near-field pore fluid is the water existing in the repository near field having been conditioned to high pH by the vault backfill). Other radionuclides (e.g. many actinides) will be solubility-limited and will be present as both solid and solute. Hence limitation of solubility is a major constraint on release from the engineered barriers for those radionuclides present in sufficient quantity in the initial waste inventory to attain chemical equilibrium between radionuclide-bearing solids (either those initially present in the wasteform or those precipitated from interactions with the near-field pore fluid) and the near-field pore fluid [33].

Due to the general absence in the mid 1980’s of solubility data for safety-relevant radionuclides at elevated pH, Nirex has undertaken a major experimental and modelling programme over the last 15 years to acquire solubility data under repository-relevant conditions (elevated pH, low partial pressure of carbon dioxide, presence of organic degradation products). Solubility data for plutonium [34] technetium [35], protactinium [36], nickel [37], niobium [37], uranium [38] inter alia have been acquired through this programme. These studies have provided extensive solubility data that have been collated in a database - the Harwell Thermodynamic Database for Chemical Equilibrium Studies, HATCHES [39]. The data in HATCHES are tested against a wide variety of experimental and field data and the source of every entrance is referenced together with supporting data and a complete update history. The database is regularly reviewed and extended in the light of the most recent literature and experimental data. It has been provided to OECD Nuclear Energy Agency for use by member countries in radioactive waste studies and is updated regularly. The HATCHES database has therefore provided a solid foundation for the UK disposal programme, and has also been applied in other major repository assessment programmes in Japan, Sweden [40] and Switzerland [41].

HATCHES provides a verified database on solubility for use in modelling studies to evaluate the behaviour of radionuclides under the chemical conditions that develop within the engineered barrier system. A number of programs are available for detailed chemical modelling, most of which are widely used outside the nuclear industry. The UK programme commonly uses the HARP/HQ program which is based on the US program PHREEQE and is designed to simulate chemical reactions and predict the solubility and speciation of key radionuclides.

The solubility of many key radionuclides (actinides etc.) in near-field pore fluids is sensitive to redox potential and pH [42]. Therefore the HARP/HQ calculations of solubility are linked to the calculation of pH and redox potential in the evolving repository pore fluids.
Nirex has carried out much research to address these issues and these are discussed in more detail, below.

4.5.2 Redox potential

One effect of the corrosion of iron or steel waste containers on the chemical composition of repository pore fluids is that free oxygen will be consumed. The consumption of oxygen will lead to a reducing environment characterised by a low oxidation potential (Eh). The products of the corrosion process will participate in the subsequent maintenance of reducing conditions. A low Eh favours the lower oxidation states of redox-sensitive elements, such as technetium and the actinides. In lower oxidation states these elements usually have lower solubility.

A recent assessment of the redox potential for a Nirex-type repository [43] calculated that Eh would be held within the range -400 to -600 mV at pH 12.5 and 25 °C. The redox potential was found to be maintained as a consequence of the redox chemistry of iron and uranium. A simple estimate of the duration of reducing conditions was also provided by this study. Based on the quantities of iron and uranium expected in a Nirex repository, and for a typical groundwater flow, the work suggested that reducing conditions may be maintained in the repository environment for at least a million years.

4.5.3 pH buffering

The NRVB is composed of a mixture of Ordinary Portland Cement (OPC) together with hydrated lime (calcium hydroxide) and fine limestone flour (calcium carbonate) [44]. This backfill is designed to condition inflowing groundwater to a high pH, and to have an extensive pH buffering capacity that will maintain these conditions for an extended period of time [45] (Figure 4.5).

*Figure 4.5 - pH evolution of the engineered system (schematic)*

Many radionuclides have low solubility under conditions of high pH [34]. Processes that might lead to a reduction of the pH buffering capacity of the NRVB have been the subject of extensive research by Nirex. These processes include the following.
• Groundwater leaching: the calcium content and pH of inflowing groundwater would be lower than that for water in equilibrium with the NRVB, so the NRVB would begin to dissolve once groundwater ingress and movement through the near field occurs.

• Reaction with acids: organic material in waste packages will decay to produce carbon dioxide, low-molecular-weight organic acids, and hydrochloric acid (the last arising from the radiolysis of chlorinated organic polymers such as polyvinylchloride). These acids will tend to neutralise a proportion of the alkalinity of the backfill [45, 46].

• Pozzolanic reactions: pozzolanic reactions involve the reaction of calcium hydroxide in the NRVB with silica in other near-field materials, notably the waste encapsulation grouts, to form CSH gel. Although the reaction is detrimental in the sense that during the earlier stages of repository evolution it will remove calcium hydroxide, the CSH-gel product can extend the period of long-term pH buffering [45].

• Cracking: crack propagation in the backfill may alter the extent to which flowing groundwater (predominantly in the cracks) is buffered to a high pH [45]. Additionally, the poorly crystalline, hydrated calcium silicates (CSH-gels) that are present in freshly hydrated cementitious materials are metastable with respect to more crystalline solids, similar to natural minerals [47]. Therefore, the cementitious materials present in the repository will tend to become more crystalline with time and this will tend to lower the pH at which the pore water is buffered. The process of crystallisation will be accelerated by temperature, which will depend on the thermal evolution of the repository following closure. The impact of alteration due to phase instability has been investigated for a range of CSH-gel compositions to ascertain the effect on the pH of water in contact with the resulting materials [48].

From this it is clear that a wide range of tests has been carried out to demonstrate the suitability of the NRVB for high pH buffering over an extended period of time. Nevertheless, it is acknowledged that the use of high pH conditions to provide large scale and long-lived chemical containment is a fairly recent innovation and it is anticipated that work will need to continue to build confidence in the concept. This will entail further laboratory testing, including some at a larger scale than has been carried out to date, and the continued search for appropriate information from natural and anthropogenic analogues so that multiple lines of evidence can be brought into play.

4.5.4 Sorption

Sorption encompasses a range of mechanisms by which the mobility of radionuclides may be retarded both within the repository on engineered barrier materials and in the far-field on flowpath surfaces.

Sorption involves the interaction between species in solution and solid phases in contact with the solution, i.e. a surface process. Sorption encompasses a range of mechanisms which result in the uptake of solute onto the solid: ion-exchange, physical adsorption and mineralisation. Generally, ion exchange and physical adsorption are fast, reversible reactions, whereas mineralisation is comparatively slow and irreversible.

Nirex has conducted a large research programme to investigate sorption processes not only on cementitious barrier materials, but also on potential repository rocks such as clays and strong fractured rocks (principally Sellafield basement rocks). These studies include those reported for high pH conditions [37, 49, 50]; those for a variety of rock types [51], those for clay [52, 53, 54, 55, 56, 57] and those for rock samples from Dounreay and Sellafield [58]. The effects on the sorption and solubility of radionuclides of species formed by the
breakdown of organic materials present in the wastes have also been studied extensively by Nirex and are discussed below. Additionally, there has been extensive work on sorption processes conducted internationally.

Empirically, sorption can be represented by a distribution coefficient (Kd) that represents the partitioning of a radionuclide between a liquid (e.g. repository pore water, groundwater) and adjacent solid surfaces. This distribution coefficient is different for different radionuclides and will vary with differing chemical conditions. The various programmes of work on sorption processes have enabled the derivation of sorption distribution coefficients for many radionuclides under many different chemical conditions [59]. Compilations of sorption data are now available for use in modelling the impact of sorption on radionuclide migration through the engineered barrier system. National programmes have developed a range of techniques to support performance assessments for a number of different concepts in a range of different chemical environments. Furthermore, the Nuclear Energy Agency (NEA) of the Organisation for Economic Co-operation and Development is currently undertaking an exercise to synthesise and evaluate data and modelling techniques used internationally to simulate sorption processes. It is expected that this work will build consensus (and hence confidence) in the ways that sorption is modelled in performance assessments.

4.5.5 Anion exclusion

When considering the form of dissolved radionuclides, four categories of aqueous species may be defined: cations; anions; neutral species with no overall electrostatic charge; and radionuclides that have formed a complex with organic material (referred to as complexes for short). If the dissolved radionuclides carry a negative charge, a proportion of the backfill porosity may not be accessible to them [30]. This effect is called ‘anion exclusion’.

Experimental studies of the mass-transport properties of cementitious materials [30] suggest that in the case of iodide ions, only around a fifth of the total pore volume of pristine NRVB may be accessible, whereas neutral and cationic aqueous species may have access to almost all the pore volume. The observation is based on comparing the porosity inferred from the measurement of the rate of diffusion of iodide ions with the measured porosity obtained from mercury intrusion porosimetry. It is a reasonable assumption that the behaviour of other effectively non-sorbing anionic species such as chloride, pertechnetate, selenate, etc. would be similar to iodide, although some variations would be expected to arise as a function of variations in charge density. For key contributors to potential calculated radiological risk, such as chlorine-36, this process of anion exclusion will lead to faster transport than a case where exclusion was not considered.

4.5.6 Colloids

The sorption of radionuclides to mobile colloidal particles (that is particles in the size range 1 to 1000 nm, Figure 4.6) that may be present in both the near- and far-fields has been identified as a mechanism that could increase the rate of radionuclide transport to the biosphere. Colloidal particles (consisting, for example of mineral fragments or bio-organic debris) are present in all natural water systems, including deep groundwaters. Colloidal particles may also be generated in the near field by the disintegration of near-field materials and formation of cement phases. Owing to their large surface-area to volume ratio, colloidal particles may have a significant capacity for radionuclide sorption. If radionuclide-bearing colloidal particles are mobile in the near field the source term flux could be increased. Furthermore, sorption of radionuclides onto mobile colloids in the groundwater may lead to lower retardation of the radionuclides as they travel through the geosphere. Therefore, colloid-facilitated transport is expected to have most impact on
radionuclides with low solubility in the near field and a strong tendency to sorb, such as the actinides.

*Figure 4.6 - Colloid size range and migration processes*

The most likely sources of colloidal material in a L/ILW repository are the cementitious backfill and wastes themselves. Previous studies have established that cement-derived colloids can form under repository conditions and can associate with radionuclides. In sorption experiments involving cementitious porewater, the presence of colloidal material associated with certain elements (zirconium, uranium, americium) has been identified by Nirex; filtration using successively smaller filter pore sizes demonstrated a range of sizes down to the smallest filter size of 2 nm. This low extreme is smaller than the pore openings...
of backfill materials (about 450 nm) [60]. It is unlikely, however, that cement colloids would be stable in changing pH conditions.

Natural inorganic siliceous colloids have a typical concentration of $10^{10}$ particles per litre with sizes in the range 40 to 1000 nm and have either negative or neutral overall charge. Experiments have shown that such colloids will tend to precipitate from the aqueous phase at the levels of calcium present in cementitious porewater [61, 62]. Natural colloids are discussed more extensively in Section 5.

4.5.7 Degradation of organic materials

One of the most important potential influences on the chemical barrier arises from the degradation of organic material in L/ILW, in particular cellulosic materials such as paper, cardboard, fibre-board and wood [29]. The degradation of some organic wastes produces organic compounds that are soluble in water. These are often described as ‘complexants’ or ‘ligands’. These organic complexants can associate with dissolved radionuclides. The organically complexed radionuclides produced by this association can have different chemical properties to those of the radionuclides when the complexants are absent. Importantly, the solubility and sorption properties of the dissolved radionuclides can be affected, with consequences for the release of these radionuclides from the repository. Solubility is expected to be increased and sorption onto the backfill reduced.

The main features of the chemical degradation of cellulose can be explained by examining a simplified representation of cellulose that treats it as an isolated chain built up from linked molecules of glucose. The main degradation process in the repository is the anaerobic, alkaline hydrolysis of this glucose chain [63]. A consequence of the degradation process is that the molecules at the end of the chain are successively removed, but in a chemically altered form to that of the original glucose. A number of water-soluble species are produced as a result of the degradation of cellulose under alkaline conditions. They may be referred to as cellulose degradation products (CDP), and have been shown to include 2-C-(hydroxymethyl)-3-deoxy-D-pentonic acid (iso-saccharinic acid, ISA).

The actual process of degradation is more complicated than this simple description, with competing reactions occurring that can affect the overall rate at which the degradation process proceeds [29]. Furthermore, the cellulose in the waste is considered to consist of two forms: amorphous and crystalline material. The amorphous material is believed to degrade much faster than the crystalline form, the former probably degrading completely over the timescale of typical laboratory studies. The rate of degradation of cellulose is an important determinant of the concentration of complexing ligands, and it is planned to carry out experiments to determine this.

The impact of cellulose degradation products and iso-saccharinic acid on the chemistry of plutonium has been a particular focus of work by Nirex: in effect, using plutonium as a model element. The behaviour of other elements, such as nickel, technetium(IV), tin(IV), thorium, uranium((IV) and (VI)), and americium, in the presence of cellulose degradation products has also been investigated [64, 65], though not in so much detail. While this work has highlighted the importance of ISA as a complexing ligand, it is possible that cellulosic degradation products may contain other important complexants.

4.5.8 Alkaline disturbed zone (‘ADZ’)

The extensive use of cement and concrete in the construction of geological repositories for low and intermediate-level radioactive wastes, both for structural, and encapsulation and backfilling purposes, requires that the compatibility of such materials with the geological environment should be addressed. Saturation of cementitious materials with groundwater
will occur in the post-closure period of disposal, producing a hyperalkaline pore fluid with a pH in the range 10 to 13.5. These pore fluids have the potential to migrate from the repository according to local groundwater flow conditions and react chemically with the host rock. These chemical reactions may affect the rock’s capacity to retard the migration of radionuclides released from the repository after the degradation of the waste packages. The effects of these chemical reactions on the behaviour of the repository rock as a barrier to waste migration have been investigated in an extensive (10+ years) research programme by Nirex for the purposes of assessing the safety of the repository design. This research programme has involved laboratory experimental studies e.g. [66, 67, 68]; modelling work e.g. [69, 70], and an in-depth investigation of a natural occurrence of hyperalkaline groundwaters at the Maqarin analogue site in northern Jordan e.g. [71] (Figure 4.7).

Figure 4.7 - Calcium carbonate formation at Maqarin (Jordan) caused by the reaction of highly alkaline groundwater with carbon dioxide in the air.
From these studies, a number of key processes affecting radionuclide migration have been identified, which could be perturbed by the migration of a hyperalkaline pore fluid plume. These include: the porosity and permeability properties of the host rock; precipitation and co-precipitation behaviour of radionuclides; radionuclide sorption; diffusion of radionuclides into dead-end pore space (‘matrix diffusion’); and colloid stability and mobility. Further, in some geological environments, alkaline disturbance could release organic materials from the host rock, and in repositories where bentonite is used, the behaviour of bentonite in contact with cementitious materials could be significant.

A good understanding has been developed by Nirex of the minerals that are likely to form in the ADZ and the controls on their stability. Calcium silicate hydrate (CSH) phases are likely to be the dominant products of cement-rock reaction. Zeolites are likely to form further from the repository. Alkaline water-rock interaction may lead to pore opening or pore closing. However, the dominant effect is expected to be a reduction in porosity. The main circumstance giving rise to pore opening is the interaction of rocks low in calcium with relatively low calcium waters such as so-called ‘early’ cement pore fluids. These fluids contain significant quantities of sodium and potassium and they would be the first fluids to be leached from the backfill. The spatial extent of the ADZ is likely to be controlled by a combination of chemical and physical processes dependent, like the porosity changes, upon (site-specific) mineralogy and groundwater chemistry. Nonetheless, the expectation is that the net effect of the ADZ will be beneficial in terms of performance assessment in that fluxes of groundwater through the near field will be reduced as a consequence of pore sealing. It is also probable that sorption will tend to be increased by alkaline reactions [72], again benefiting safety.

4.6 The effects of gas generation

Gas could be formed following closure of a repository in quantities that are of potential significance to the assessment of post-closure safety. A range of gases may be generated within the repository:

- hydrogen may be generated by the corrosion of metals in wastes and packaging;
- methane and carbon dioxide may be produced by microbial degradation of cellulosic material in wastes, mainly wood and paper; and
- hydrogen sulphide may be generated in small quantities from microbial action on sulphate ions in wastes and groundwater.

Traces of three other categories of gas might also form:

- radioactive gases might form, in particular tritiated hydrogen (³HH), ¹⁴C-labelled methane (¹⁴CH₄) and ¹³C-labelled carbon dioxide (¹³CO₂);
- radon could be formed by the radioactive decay of uranium, thorium and radium; and
- other toxic non-radioactive gases might form as the result of microbial processes.

The engineered barrier system is designed to permit the migration of these gases. Gas pressure within the engineered barrier system may build up sufficiently to allow the movement of the gas into the surrounding rocks. There is a possibility that the gas pressure may build up sufficiently that it can disrupt the surrounding rock by the creation of additional fractures. The issues created by the generation of the gas in a repository will vary depending on the rate of gas generation, the rate at which gases can dissolve into
groundwater and the rate at which it can dissipate through the repository and surrounding rocks [73].

Research into gas generation and migration is being carried out in a number of countries and as part of international collaborative exercises. The emphasis of different gas research programmes vary with different repository designs. There is therefore a fairly comprehensive range of knowledge that takes into account different design concepts and host environments. In some countries, there are comprehensive programmes of research aimed specifically at providing the models and data necessary to support repository performance assessments [74]. Nirex has contributed to the development of this knowledge base by extensive gas research programmes, focussed on the development of methods that can be used with confidence to model gas generation within a repository.

The computer program GAMMON [75] has been developed to model the generation of hydrogen, carbon dioxide, methane and hydrogen sulphide by corrosion of metals in wastes and by the microbial degradation of organic wastes (Figure 4.8). Solid-state diffusion may result in the release of tritiated hydrogen from the waste steels and this process is also considered within the program. GAMMON is based on a considerable research programme conducted by Nirex to investigate gas generation in the engineered system and documented in a number of Nirex reports [73, 76, 77].

The research into this area has comprised a combination of theoretical and experimental work. This work shows that the largest single source of gas in a repository will be anaerobic corrosion of steel present in wastes and as packaging [78]. For this to occur, it is first necessary for the oxygen in the air trapped in the vaults at closure to be consumed by aerobic corrosion and microbial processes [73]. Experimental work involving carbon and stainless steels embedded in cement, or immersed in the high pH water that results from equilibration with cement, shows that the rates of anaerobic corrosion are expected to be very low under repository conditions: around 1 \( \mu \text{m yr}^{-1} \) for carbon steel [79] and below 0.1 \( \mu \text{m yr}^{-1} \) for stainless steel [80]. Certain other metals, including Zircaloy, Magnox and aluminium, have the potential to generate significant quantities of hydrogen, even in the presence of oxygen. The corrosion rate of zirconium alloy has been found to be very low under simulated repository conditions [81]. However, Magnox and aluminium can potentially corrode relatively rapidly [82].

It is important that the methods developed to evaluate gas generation can be used with confidence. For the major gas, hydrogen, which is mostly produced by the anaerobic corrosion of steels, this is, for the most part, a fairly simple question of correctly estimating the corrosion rate and combining this with the mass and surface area of the steel. For the gases produced by microbial action, however, the situation is very much more complicated. Here, the rate and mass of gas produced depend upon the types and numbers of microbe initially present and the way that these change under the influence of the environmental conditions.

The ability of the GAMMON program to model these complex microbial processes has been subjected to a validation process. For example, GAMMON was used to predict the cumulative volumes of gas generated in twelve drums containing simulated LLW under a variety of moisture and pH environments. The drums were buried underground and the gas composition and generation rates were monitored continuously over a three year period. Comparison of the measured data with modelling results from the GAMMON program [78] were partially successful, although the data were not sufficient to gain complete confidence in the ability of GAMMON to calculate microbial gas generation under repository
Figure 4.8 - (a) Gas generation rates after repository closure and (b) cumulative amounts after repository closure
conditions. Further work has been undertaken to provide a more comprehensive dataset with which to test the validity of GAMMON.

The vast majority of this research regarding the generation of gases from the repository would be directly transferable to different sites, as it is determined by the nature of the wastes and the design of the engineered barrier systems.

4.7 Criticality

The disposal of radioactive waste will often entail the disposal of some fissile radionuclides, i.e. radionuclides that, given certain conditions and a sufficient mass of the fissile isotope, have the potential to cause a critical chain reaction involving the production and capture of slow neutrons. The most significant fissile radionuclides in the UK inventory are plutonium-239 and uranium-235.

By applying a limit to the amount of fissile material that may be contained in a waste package, it is possible to ensure that, so long as the fissile radionuclides are confined to the waste packages, no criticality will occur. This assurance will apply for any credible configuration of the waste packages and for any conditions that could occur during waste storage, transport and emplacement in the repository. However, in the long term, after deterioration of the physical containment provided by the waste packages, the possibility arises of movement of fissile material out of the waste packages and subsequent accumulation into new configurations that could, in principle, lead to a criticality.

The issue of post-closure criticality has been studied in a number of countries including the UK, Sweden, Germany and the USA; see [83]. A focus of the research has been the examination of the natural analogue provided by the naturally occurring nuclear reactors discovered at Oklo in Gabon in west Africa in 1972. The nuclear reactions there started about two billion years ago and lasted for about one million years. Two billion years ago natural uranium contained about five times more uranium-235 than it does today so that, unlike at the present day, it was then possible to create a water-moderated reactor using natural uranium alone. Uranium ore bodies often give opportunities to study the mechanisms by which fissile material (uranium in this case) might be accumulated, but at Oklo the opportunity also arises to study the mechanisms by which a natural criticality might be sustained and the consequences of this occurrence.

Nirex has produced a report [83] that summarises its work over the period 1992 to 1998 on developing the understanding, data, models and methods necessary to assess post-closure criticality safety. Work on the possible effects of a criticality, were one to occur, and its impact on repository performance is also summarised. In summary this work shows that the accumulation of sufficient fissile material to give a criticality is unlikely to occur in a repository. It also shows that in the unlikely event that a criticality were to occur, it would be a localised event and would have a negligible effect on the capacity of a repository to continue to contain wastes safely. The work shows how controls on the placing of waste fissile materials in well-engineered packages and on their subsequent emplacement in a repository would limit the chance of a criticality.

4.8 Summary of knowledge and capabilities

Much work has been undertaken on the following key topics for waste immobilisation and migration: metal corrosion; gas generation; radionuclide solubility and sorption; colloid generation, stability and mobility; and the alkaline disturbed zone. For the most part, this research base could be transferred to the design and construction of a repository with a
cementitious near-field anywhere in the UK. However, in the United Kingdom, some of this work has been rock-type specific (e.g. investigations of alkali-rock reaction relating to Sellafield basement rocks) and therefore would need to be developed further for other potential geological environments.

Repository programmes for ILW and LLW are well advanced in Finland, France, Sweden, Switzerland and the USA, with underground repositories already in operation in Finland, Sweden and the USA. Various designs are adopted that use different engineered barrier systems. In the United Kingdom, the use of backfill other than cement, such as bentonite or crushed salt, would require further research, although much relevant information could be obtained from research programmes conducted elsewhere (e.g. Sweden, Switzerland, Germany). A similar position would exist for alternative repository designs, using for example, lined tunnels rather than free-standing rock vaults. The Nirex research programme concerning the use of cementitious engineered barriers in both clays and strong fractured rocks places the UK in a sound position for the future design, location, and construction of a repository for the geological disposal of intermediate level radioactive wastes.
5 CHARACTERISING THE GEOSPHERE

This Section summarises research into the geosphere, and in particular discusses the role of site characterisation. The geosphere is defined on page 2.

5.1 The role of the geosphere

An obvious but nonetheless fundamental point is that a repository has to be capable of being constructed and, while it is possible to make underground openings in virtually any rock type, the competence of the host rocks will profoundly affect repository design. This aside, the geosphere also needs to ensure low groundwater flow into and through the repository and provide conditions (particularly chemical conditions in the groundwater) that do not adversely affect the engineered system. Other important geosphere characteristics are a long travel time for groundwater to move from the repository to the biosphere and retardation of radionuclides relative to groundwater flow. These factors help provide a long travel time for radionuclides to move through the geosphere, giving time for them to decay and disperse within the system. This reduces the amount of radionuclides released into the biosphere at any given time. A final important geosphere characteristic is the natural attenuation of radionuclide concentrations in groundwater by dispersion and/or mixing with other groundwaters along the flow path.

Key questions in researching the geosphere are therefore the amount of groundwater moving through the repository and its surrounding environment, its rate of movement and the pathways taken back to the biosphere. The transport process affecting solutes entrained in the groundwater also need to be understood. It is also important to understand the level of protection provided by the geosphere as a radiation shield, against the chemical degradation of the engineered barrier system, and the disruption of the engineered barriers by natural and man made events. The migration of radionuclides in gases produced within the repository is another means of radionuclides returning to the biosphere, and therefore an understanding of gas migration through the geosphere is required. These key questions are illustrated in Figure 5.1, together with important contributing factors. These issues are all, in part, determined by the geological, hydrogeological and geochemical properties of the rocks that make up the geosphere. Issues of particular importance are listed below.

- The properties of the rocks in the geosphere, in particular permeability and porosity, which are determined by the fabric of the rock, in particular the nature and variability of the void spaces in the rocks.
- The chemical and mineral properties of the rock and groundwater. These will affect the concentrations of radionuclides in the groundwater and may also affect the chances of human intrusion.
- The hydrological processes and conditions existing within and around the rock mass. These processes and conditions determine the driving forces for groundwater movement and the amount of recharge to the groundwater flow system. These control the boundary conditions and hydraulic head distribution within the geosphere, and create the potential for groundwater movement.

These properties will vary from rock type to rock type, and will vary for similar rock types in different locations. Site-specific studies to characterise these properties (site characterisation) therefore form a very significant component of research into the geosphere.

Most of the required functions of the geosphere are enhanced by positioning the repository at some depth below the surface. This provides large volumes of rock between the
repository and the surface, which provide greater opportunities for solute retardation, and also increases the time for the movement of gas and groundwater through the geosphere back to the biosphere. At depth, the groundwater system is generally relatively stable and is less responsive to processes operating at the surface. The chances of disruption by natural events and anthropogenic activities are therefore reduced. On the other hand, the positioning of a repository at depth increases temperature, rock stress and the difficulty of access. It will also increase the difficulty of characterising the site-specific properties. Therefore, the ability to characterise the geosphere at a particular repository location is also an important issue to consider in any geosphere research programme.
The geosphere is highly influential in determining the performance of a repository. Different disposal concepts and geological environments place different weighting and functions on the engineered barrier system and on the natural, geological barrier. The weighting depends on the relative importance of factors such as physical containment of the wastes, chemical conditioning around the repository, protection of the engineered barriers, and retardation and dilution of releases. For example, as concepts have developed for fractured rock environments, research and performance assessments have explored the range of behaviours and interactions of the various components of disposal systems (see, for example, [84]). Protection of the engineered barriers is increasingly seen as an important function. In addition, the different functions of the geosphere will change in importance with time.

One of the most immediate functions is non-technical. Emplacement of the wastes in a stable underground repository (whether with direct closure or a provision for long-term retrievable underground storage) is one of the few options capable of meeting the modern requirements of sustainability and inter-generational equity [85]. Responsible management of the wastes is a matter for those who have benefited from their production and not a problem which ought to be passed on to future generations. The massive rock barrier, as a component of the repository system, provides a visible and solid sign that the task has been addressed with proper regard to removing the wastes from the human environment.

The primary technical functions in the early years after disposal (a few hundred to a few thousand years) are those of providing a simple radiation shield and removing the wastes from the human environment. In all deep repository concepts, much of the protection afforded by the system over several hundreds of thousands of years comes from chemical interactions of radionuclides within the evolving engineered barrier system. Thus, ensuring that the engineered barrier system evolves undisturbed throughout this period is the key function of the rock.

Also on the hundred thousand year timescale, the rock affords a significant retarding role for the longer-lived radionuclides that have escaped the engineered barrier system rather than having decayed in situ. By this time, these are principally the natural uranium decay series radionuclides and activity levels in the repository are, in any case, approaching those of natural background or, in the case of spent fuel or depleted uranium disposal, a uranium ore deposit. The main period of potential hazard was much earlier in the life of the system. This generalised picture varies in detail from one geological environment and engineered barrier design to another, and from waste to waste and radionuclide to radionuclide, but is nevertheless a useful indicator of what the disposal system might be designed to achieve.

Some radionuclides are significantly mobile once released into a groundwater system (e.g. iodine-129 and chlorine-36) and both the geological barrier and the degraded engineered barriers have limited capability to retard their movement. It can be seen, however, that in some concepts there is a significant role for the geological barrier to attenuate such releases by dispersion and/or dilution in other groundwaters along the flow path. In this way eventual releases are at concentrations that fall below levels of concern.

5.2 Groundwater movement through the geosphere

The geosphere is a key factor affecting the groundwater flow pathway for the return of radionuclides to the accessible environment. Groundwater flow will occur along many different routes back to the biosphere. As groundwater from the repository moves into the geosphere it will spread out within the rocks as a plume, mixing with groundwater that has
not flowed through the repository. The distance over which the groundwater travels from
the repository to the surface is called the path length (Figure 5.2).

Figure 5.2 - Schematic illustration of the groundwater, gas and human intrusion
pathways

It is determined by the location of the repository and the overall groundwater flow field (the
pattern and rate of groundwater flow). The groundwater flow field is determined by the
properties of the groundwater (e.g. density and viscosity, which in turn depend on
temperature and salinity), the properties of the rocks (which determine the resistance to
groundwater flow) and the forces driving the flow. Radionuclides in solution, and those
entrained as colloids or particulates will be carried along with the flowing groundwater.
This process of transportation (advection) is the predominant mechanism by which
contaminants move through most geological systems. A general understanding of groundwater flow at a site is therefore fundamental to understanding the containment properties of the geosphere at that site.

The average time for groundwater to travel from the repository to the biosphere depends on the path length and the speed at which groundwater travels along the path. The amount of groundwater moving through a given area in unit time is called the groundwater flux. The groundwater flux depends on the physical properties of the rocks, in particular the permeability, a measure of the ease with which groundwater can move through the rock and the flowing porosity. The permeability depends on the geometry of the void space - the size, shape and connectivity of voids within the rock mass (the porosity). Flowing porosity arises from void spaces that are connected together in a way that can permit the movement of groundwater.

Groundwater travel time decreases as the groundwater flux in the geosphere increases, which can generally be related to an increase in permeability. For any geological environment, porosity and permeability will vary within and between different rock types. There will therefore be a range of travel times for groundwater moving from the repository to the surface within any single given geological setting. The spatial variability of these key properties of the rocks are therefore important in determining the rate of groundwater movement. In addition, the presence of features within the rock mass that cut across the geological formations and can act as groundwater pathways with short travel times can significantly affect the general containment properties of the geosphere.

The groundwater flow system at a site changes as the site evolves over geological time periods. Climate changes can affect the processes driving groundwater flow and geological processes such as erosion and sedimentation can affect the properties of the host rock. These processes will act on the system over the time periods of interest for long-lived radioactive wastes. Time dependency is therefore an important consideration in understanding groundwater flow. One of the reasons for siting a repository at some depth below the earth’s surface is to remove the repository from the shorter term effects that climate change can have on the groundwater flow system. Groundwater flow regimes at depth are often isolated from a more active groundwater system that occurs nearer the surface in response to hydrological processes at the surface. Indications of long-term stability in the groundwater system can therefore be used to establish the level of isolation from surface processes that can be expected.

5.2.1 Understanding groundwater flow

Because of the significance of the groundwater pathway, a key step in evaluating the performance of a potential repository system is to develop an adequate understanding of groundwater flow at any potential site. Groundwater flow models represent this understanding and enable contaminant transport to be calculated. In order for there to be confidence in these models, they need to be founded in site-specific information on the geology and hydrogeology of the site. Site characterisation provides the necessary geoscientific information (geological, hydrogeological, geochemical and geotechnical). This information is used to develop conceptual models of groundwater flow at the site, and hence provide the basis for evaluating risks from radionuclide migration in groundwater at the site. Such evaluations are required at various stages of a repository development programme (Figure 3.3).
The extent of site characterisation and groundwater flow modelling required for evaluations of the site depends on the type of disposal facility under investigation, the regulations governing the licensing of the facility and the particular stage in the siting process that is being addressed. An important factor in the licensing of a facility for the geological disposal of radioactive wastes is the very long timescale over which safety needs to be assessed. Over such long timescales, natural and anthropogenic processes and events will change many components of the repository system. The geosphere and biosphere will respond to climatological and geological changes, causing evolution in the groundwater flow path and interactions with the repository near field. It is therefore important to characterise the geosphere in its present state, and to understand how it has evolved in the past. Geoscientific information from site characterisation may be used to develop conceptual and numerical models of the behaviour of the current groundwater system, its past evolution, the possible sequences of events which could occur in the future, and their consequences for the evolution of a radioactive waste disposal facility.

The confidence with which groundwater flow models can be used is, in part, dependent on the process adopted to develop those models from site-specific data. It is important that there is constant iteration between the data on which understanding is founded, the models that represent that understanding, and the experts involved in both. It is also important that the fitness for purpose of the models is clearly established. Therefore, groundwater flow models are usefully developed by a process that adopts a series of iterative steps. As shown in Figure 5.3, these steps begin with the acquisition and interpretation of data. Following this is the processing of data to produce first a conceptual model and then a numerical flow model. Construction of the numerical flow model will require parameters that were acquired at the metre-scale and tens-of-metres-scale to be modified (upscaled) so that they represent rock properties on a hundreds- or thousands-of-metres-scale. The model is then calibrated using experimental data (e.g. borehole pump test results) and site data (e.g. natural salinity and temperature gradients). The groundwater flow model can then be used to calculate the movement of radionuclides so that, ultimately, an estimate of radiological risk can be obtained.

Figure 5.3 - Iterative process of groundwater flow model development
All potential disposal environments, in whatever rock type, will be associated with geological complexities at all scales; this is an inevitable consequence of dealing with natural systems. Uncertainties regarding the geological environment are likely to remain in some areas, even after an extensive site characterisation programme. Given the many functions and the importance of the geosphere barrier, it is particularly important to characterise the geosphere to a sufficient standard. This will have been achieved when it is clear that the residual uncertainties have an insignificant impact on repository performance.

A number of issues are currently of central interest among those concerned with geosphere investigations around the world. Several of these have arisen as a result of applying an iterative approach to performance assessment and site investigations over the last ten years. The most important topics currently receiving attention are:

- the identification and characterisation of the way that the in rock and groundwater properties vary over distance (known as spatial variability or heterogeneity) and the ability to make adequate estimates of geosphere properties and behaviour at various length scales from limited sets of data;
- the identification and characterisation of potential fast groundwater flowpaths through the rock, including those produced by excavation disturbance;
- the capability to demonstrate that deep groundwater flow and chemistry is stable over long periods of time, despite major changes in the surface and near-surface environment; and
- the identification and characterisation of time-dependent processes which affect the evolution of the geosphere: i.e. processes which are cyclical or generally not constant over the time period of interest for waste containment.

Each of these issues is discussed separately in the following sub-sections.

### 5.2.2 Spatial variability

All natural systems are spatially variable. The extent of this variability and its characterisation and representation in modelling affects calculations of geosphere performance. An understanding of the spatial variability of properties such as rock quality, porosity and permeability is important to support repository design (in particular construction options for an underground repository) and to understand the hydrogeology and develop a better understanding of groundwater flow. Spatially variable systems can offer the potential for a large amount of dispersal, which can be significant in terms of groundwater travel times and pathlengths and solute transport.

However there is normally also a significant degree of uncertainty regarding the spatial variability of geological formations. The investigation of rocks at depth imposes limitations on data gathering, and, while an underground facility will resolve many issues, some of these uncertainties will, below a certain level, be irreducible. In general, greater confidence can be gained for geological and hydrogeological environments that are amenable to simple representations, i.e. an environment in which spatial variability is understood and quantifiable.

The subject of spatial variability may be most significant for fractured rocks, in which the heterogeneity of the hydraulic and transport system can be particularly marked. However, the extent to which it is possible to identify sites with minimal spatial variability in geological properties is unknown. During a site selection process, little geological information will be available concerning the rocks at depth. Therefore, it may be impossible to identify such sites with any confidence ahead of detailed investigation.
Nirex, in common with waste disposal agencies in other countries, has invested considerable effort in examining the spatial variability of the geological environment [86] during detailed investigations. The work at Sellafield included not only the investigation of the spatial variability of the rock mass itself, but also the fluid chemistry, the hydrogeological system and the physical factors which influence groundwater flow [26]. The structure and hydrogeological properties of the rocks and the glacial sediments were also investigated for the purpose of performance assessment [12]. Several different methods were used to apply and integrate the data that had been obtained from the testing of rock cores, from borehole wireline logs and from seismic acoustic impedance data obtained from a trial 3D seismic survey (Figure 5.4). It was concluded that the work demonstrated the feasibility of determining rock mass properties throughout a volume of rock relevant to geotechnical and hydrogeological aspects of an underground repository [87].

**Figure 5.4 - Downhole logs indicating the spatial variability of different properties in Borehole RCF3 at Sellafield, Cumbria.**

<table>
<thead>
<tr>
<th>Property Type</th>
<th>Depth Interval (meters)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wireline property log</td>
<td>-800 to -600</td>
</tr>
<tr>
<td>Stony wave reflection coefficient</td>
<td>-650 to -600</td>
</tr>
<tr>
<td>Zones of measured inflow (no magnitude implied)</td>
<td>-700 to -650</td>
</tr>
<tr>
<td>Potential flowing features</td>
<td>-750 to -700</td>
</tr>
<tr>
<td>Short interval test</td>
<td>-750 to -800</td>
</tr>
</tbody>
</table>
The subject of spatial variability and how it should be modelled is of great interest in the assessment of mineral reserves and in the oil industry. In the latter, it is the 3-D structure of the reservoirs that is of most interest and much research has gone into ways in which a reservoir could be investigated and modelled [88]. Upscaling from local borehole data, combined with much larger-scale seismic data has been used to try to incorporate the spatial variability of the rock mass at all scales so that the 3-D structure of the reservoir is realistically modelled [89]. Similarly, in radioactive waste disposal research, spatial variability has most frequently been considered in terms of the structure of the rock mass. Investigations in Canada, Sweden, Finland and Switzerland have investigated the structural heterogeneity at all scales, from the scale of regional fracture zones to those at the block scale of a few metres and down to the scale of single fractures. The spatial variability of the geochemical environment, including the variability in groundwater chemistry and the alteration of the rock mass has been less frequently considered.

The groundwater flow system in low permeability fractured rocks tends to be controlled by the spacing of the most hydraulically significant fracture zones, often on the scale of a few hundred metres. Because of the variability of the rock mass, the identification of these hydraulically significant fracture zones is difficult. Multiple lines of evidence need to be considered, to develop an understanding of the nature of groundwater flow through the rock mass that is self-consistent with data from mapping at surface, core logging, geophysical testing at surface and downhole, hydraulic testing within boreholes and mineralogical and geochemical evidence of past groundwater flows (for example calcite mineralisation in fractures).

At Sellafield, extensive effort was put into the multidisciplinary interpretation of such data sources [86, 26] with the result that features were identified that had the potential to flow (potentially flowing features or PFFs). These PFFs were fractures that contained late calcite mineralisation (indicating the passage of groundwater) and open porosity (indicating a continued potential for groundwater flow). There was a correlation between these PFFs and the location of zones of inflow into boreholes (Figure 5.4). In some localities, these PFFs were clustered, and it was these clusters of PFFs that were interpreted to act as the most hydraulically significant fracture zones. This understanding was built into the conceptual model for groundwater flow used in the Nirex 97 assessment [12]. A key uncertainty remained regarding how these PFF clusters connected together within the host rock formation. This was addressed by evaluating three different conceptual models (Figure 5.5).

In general terms, methods exist to allow the issue of variability in geological and hydrogeological properties to be adequately addressed. Some unresolved uncertainty will always remain, of course, and it is possible that at some sites this could be sufficient to produce an unacceptable level of uncertainty in the large-scale properties of the site.

5.2.3 Fast Pathways

Most rocks are almost certain to contain zones through which fluid can travel at faster rate than through the average rock mass (fast pathways). These are a particular manifestation of the spatial variability of the rock mass. They are features that could result in fast flowpaths for groundwater or gas from repository depths to the more accessible environment at or near the surface. The rate of movement along such features can be several orders of magnitude faster than through the rock mass. These pathways can, therefore, restrict access to significant parts of the geological barrier and can thus significantly affect the containment performance of the geosphere. The detection of fast pathways and the analysis of their distributions is an important and often difficult part of a site characterisation programme.
The problem posed by the possible presence of these fast pathways needs to be considered at all scales (Figure 5.6).

In fractured rocks, the difference in hydraulic conductivity between a fast pathway and the background rock (i.e. the rock lying between the more transmissive zones) could lie in the range $10^2$-$10^7$ ms\(^{-1}\). Fast pathways in such rocks are most likely to be associated with fracture or fault zones or significant fractures, but there are other structures, such as contact zones between rock types and unconformities with overlying sediments, that could also be important. There are also fast pathways that can be generated by human activities (for example, mine workings, solution collapse, boreholes).

Only a subset of the existing fractures will be significant in terms of the movement of groundwater. Not all fracture zones will be transmissive. In addition, transmissive pathways can also be formed by apparently minor fractures. Such structures play an important role in controlling groundwater flow and in defining the structure within groundwater flow models. The location and geometry of the larger fracture zones can
generally be determined with an acceptable accuracy. However, the smaller, but possibly still significantly transmissive fractures are more difficult to identify and characterise.

**Figure 5.6 - Illustration of a possible concept for flow through transmissive features in fractured rock (after Nirex 97)**

The identification, testing and modelling of such fractures in strong rocks is of current interest in Finland and Sweden. Research in the Swedish Äspö Hard Rock Laboratory has increased understanding in this field through collaborations with experts from many countries (Figure 5.7 [90]).

In sedimentary rocks and evaporites fast pathways are also present. They can be associated with fracturing, faulting and lithological boundaries, and also with large “sedimentary structures” such as folds. It is likely that a repository in a potential sedimentary disposal environment would not be associated with significant “sedimentary structures”. However, it is unlikely to be possible to avoid all these features, and relatively fast pathways in an otherwise poorly transmissive sedimentary succession are a distinct possibility. Conceptual models of low permeability sedimentary sequences often assume the presence of fast pathways e.g. Nagra’s initial conceptual model of the Opalinus Clay [91]. The oil industry has also shown a greatly increased interest in fast pathways over the last few years, e.g. [92]. Modelling of groundwater flow on the basin-wide scale often assumes the presence of more transmissive structures through low permeability sedimentary sequences in order to balance fluxes. This may be a cautious assumption - Nagra’s current investigations of the Opalinus Clay using 3-D seismics and a deep borehole suggest, for instance, that the Opalinus Clay does not possess such structures.

Major faults receive particular attention as potential candidates for fast pathways. They can be important in two respects: if fault displacement is sufficiently great, formations can be displaced such that two units with markedly different properties become juxtaposed.
This reduces the cross-sectional area for flow in the more transmissive formation, and the less transmissive formation can act as a barrier to groundwater flow.

Secondly, the properties of the rock immediately surrounding the fault can be modified to produce a zone, often at relatively high angles, which can have very different properties from that of the surrounding rock (Figure 5.8). Such a zone, however, could be more transmissive when passing through some rocks and possibly less transmissive when passing through others.

**Figure 5.7 - Schematic diagram of the Äspö single fracture experiment**

Schematic configuration of the first stage TRUE experiments. The central borehole will be opened and allowed to drain while tracer is injected in the surrounding boreholes that intersect the fracture plane. The tracer concentrations measured in the central hole will be compared to model predictions made prior to the experiment. Predictions will be based on data collected during characterisation of the test site (SKB, 1996).
5.2.4 Excavation Disturbance

Additional localised flow paths may be formed due to the construction of the repository by, for example, the development of Excavation Disturbed Zones (EDZ) adjacent to the underground openings. The extent of the EDZ will be dependent on the properties of the host rock, the \textit{in situ} stress state and the method of excavation. The EDZ will normally be largest in strong rocks. The repository itself could act as a link between fast pathways that otherwise would not be linked. For example, the separation of fracture zones or faults could be considerably less than the dimensions of the repository. However, where such structures intersect the repository they are likely to be sealed and this effect may only be minor.

Just as fractures caused by excavation disturbance can modify groundwater flow, so also can groundwater flow modify the fractures (by changing the effective stress state for instance). This is an example of a coupled process. Further, if a repository generated a significant level of heat (e.g. through the disposal of spent fuel) this could be coupled to both groundwater flow and mechanical disturbance. The modelling of these coupled thermo-hydro-mechanical effects is being undertaken by the international DECOVALEX project, now in its third phase of work. With co-operation from Nirex and its contractors, progress is being made in the mathematical modelling of these coupled processes [93]. With increases in computing power and greater numbers of well-instrumented \textit{in situ} experiments, the modelling of these effects will gradually improve. Even on the basis of current knowledge, it is possible to take steps to ensure that the most significant effects of coupled processes are avoided.

5.2.5 Demonstrating stable groundwater conditions

The ability to study the present-day hydrogeological system and relate it to past groundwater conditions (e.g. glacial events), provides a strong semi-quantitative basis for demonstrating the stability of the groundwater system and for developing scenarios of potential future changes (or lack of change). The relatively new science of
paleohydrogeology (the study of past groundwater conditions) generally relies on the examination of the chemistry of the rocks and the groundwater.

Of particular relevance are the following.

- The chemical composition and variability of fluids (e.g. groundwater in fractures and in the rock matrix, and fluids trapped within particular minerals) and the differences between the different types of fluids. This information can identify how many different types of fluids exist, how well they are mixed, whether they have originated at different times in the past and the composition of the solid phases with which they have equilibrated.

- The mineralogy of the rock surfaces accessible to groundwater, in particular the chemical composition, morphology and nature of discrete mineral phases. This information can provide information about how the chemical composition of groundwater in contact with the rock surfaces has changed over time, whether the minerals on the rock surfaces are in equilibrium with the present day groundwaters, and whether active water/rock interaction processes are occurring. Mineralogical information is particularly relevant as it can indicate groundwater flow paths through the rock mass. In fractured rocks, mineralogical data can often distinguish between actively flowing fractures and those that do not contribute to overall groundwater flow through the rock mass.

Hydrochemical investigations are therefore a necessary component of site characterisation, since they test the applicability of many of the processes on which conceptual models of the groundwater system are based. Such processes include changes in salinity and Eh with depth, the control of pH by geochemical reactions and the importance of present and past boundary conditions to groundwater movement. Hydrochemical and isotopic measurements also identify groundwater bodies that might differ in terms of their origins and relative residence times.

In addition, chemical evidence can provide qualitative information with which to support the development of quantitative numerical models of groundwater flow. This subject has recently been reviewed [94] with reference to the disposal of both HLW and ILW, using experience gained from SKB’s and Nirex’s disposal programmes, but also drawing on the experience gained in other programmes, such as those in Switzerland and Finland. In general, hydrochemistry is used to constrain the features, events and processes considered in performance assessment, e.g. geosphere evolution scenarios deduced from palaeohydrogeology, mass transport by diffusion (e.g. in clays), gas migration and dissipation. More specifically, the use of hydrochemical evidence in the following applications has been considered [94]:

- establishing flow path geometry in particular for fracture networks;
- identification of where diffusive mass transport operates in the geosphere;
- testing the self consistency of models at various scales;
- providing constraints on modelling the mobility of trace solutes (e.g. sorption, cation exchange);
- providing evidence of dilution and spreading (i.e. spatial and temporal dispersion);
- using groundwater compositions to control the densities of groundwaters at the boundaries of a flow model; the model then calculates density/salinity and head/pressure distributions within the model for comparison with observations;
testing the results of a flow models against independent chemical data (e.g. using groundwater and solute age constraints to test transit time estimations from recharge to the repository and from the repository to the biosphere - noting that steady-state modelling may be inadequate to describe the observed system);

- identifying time-dependent boundary conditions for groundwater flow models; and

- confidence building using qualitative hydrochemical evidence from natural analogues and studies of natural systems (which are playing an increasingly important role in performance assessment).

The definition of the groundwater flow paths, integral to understanding groundwater flow and its eventual link with solute transport modelling, is usually achieved by analysing information gained as part of the hydraulic testing programme. However, significant additional information can be gained by detailed consideration of open fracture mineralisation [95]. An integrated interpretation of hydraulic, hydrochemical and geochemical information will more effectively constrain the modelling of the controlling features of a site than would be achieved by reliance on hydraulic parameters alone. Even so, these techniques will often provide a range of possibilities rather than a unique model of the evolution of the site.

Integrated hydrochemical interpretations of the groundwater flow system are playing an increasingly dominant role in unravelling the complexities of the origin of the groundwater and its movement. Sellafield and Äspö are two sites where hydrochemistry has helped to constrain conceptual models for groundwater flow modelling e.g. [96, 26]. Similar hydrochemical programmes have also taken place in other countries, e.g. Finland [97].

At Sellafield, hydrogeological principles, in isolation, would describe the flow system in terms of topographically-driven flow from the high ground to the east of the site, forming an interface with the low energy saline groundwater system in the basin to the west of the site. Hydrochemical measurements (specifically Cl and Br concentrations) combined with these physical principles have enabled a conceptual model to be constructed which has considerable greater certainty in terms of the interfaces (i.e. mixing zones) between the groundwater masses and their time-dependent origins and driving forces [98]. Similarly, hydrochemical and isotopic data have distinguished various component groundwater masses at Äspö that can be represented in a hydraulic flow model (Figure 5.9 [94]).

Based on this experience, there are areas for improvement in researching the geosphere that could enhance the benefit to be gained from integrating hydrochemical data with groundwater flow models. These are:

- acquisition of hydrochemical data with the specific aim of building confidence in performance assessment models of groundwater flow; and

- providing semi-quantitative models of groundwater evolution with appropriate levels of detail for integrating hydrochemical interpretations.

These impact on the process of site characterisation and suggest that reliable, representative and realistic data are needed in areas such as those related to the interpretation of tritium and $^{14}$C data and increasing confidence in end-member compositions. This requires understanding and, where possible, minimising the extent of contamination of sampled groundwaters. An area where improvement is believed to be required is in the measurements of the pore water compositions of low permeability clays and the repository host rocks. These rocks and pore waters will be in intimate contact with the engineered
barrier system and should provide key input chemical parameters for near-field modelling calculations.

**Figure 5.9 - Hydrochemical conceptual model for Äspö Island showing groundwater flow and variations in chloride concentration**

5.2.6 Time dependency

Characterising the present condition of the site will only provide partial information for a performance assessment exercise. It is likely that one or more attributes of the site will be in a transient state. For example, in the UK it is probable that the effects of the last glaciation (Figure 5.10 [99]) will still be present to some extent at depth in many areas of low permeability rocks. In addition, sites will evolve over the time period considered for a performance assessment and this evolution needs to be taken into account. This was the topic of considerable work by Nirex at Sellafield [26].

In general, programs used in performance assessments world-wide adopt simplified representations of the behaviour of the natural system [100]. Until recently these programs have not allowed for the treatment of time- and spatially-varying system behaviour, (although supporting thermal, chemical, hydrogeological and mechanical programs often do so, and allow the definition of representative ranges to be used in steady state calculations). Therefore, there is an increasing tendency to use time-dependent programs to explore the important processes affecting groundwater flow, and adopt steady state properties for performance assessment calculations that need to take into account a wider range of features, events and processes over time. Particular attention has been focussed in several disposal programmes on time-dependent aspects of climate change and its associated uncertainties, and this subject has been of particular interest to waste disposal organisations in Europe, such as Nagra (in Kristallin-1 [101]) and SKI (in SITE-94 [102]). SKI, for example, developed a future climate sequence for their Central Scenario [103], involving ice sheet advance and retreat. SKB have been investigating the modifications to the
groundwater flow system due to climate change for many years [104]. Other time-dependent processes that have been considered in performance assessment include uplift and erosion in Kristallin-1 and the flushing of the repository near-field by oxygenated glacial meltwaters in SKB-91 [104] and Posiva’s TILA-99 [105] performance assessment.

*Figure 5.10 - Europe, 18 000 years ago (from [99] based on work from the 1980s)*

None of the performance assessment calculations used time-dependent programs - the general approach has been to apply steady-state programs and consider various future scenarios, in which the boundary conditions have been altered. Time-dependent programs need to be capable of dealing with such factors as variable boundary conditions and variable properties. This can make the programs complex and requires considerable computing time.
However, considerable attention is now focussed on the development of programs that permit the time-dependent modelling of the repository system as a whole. Nirex has been developing a capability to carry out time-dependent probabilistic modelling within future performance assessments (see Section 7).

5.3 Radionuclide transport mechanisms in the geosphere

Several processes are important in controlling the rate at which radionuclides move through the geosphere in solution or in particulate form. Radionuclides can move at substantially different rates than the groundwater which carries them. As radionuclides dissolved in groundwater move through the geosphere they can spread out. This process is called dispersion and it occurs as radionuclides in solution move through the pore spaces within the rock (Figure 5.11). Dispersion occurs in the direction of flow due to variations in pathlength through the pores and pore size (longitudinal dispersion) and perpendicular to the flow direction (transverse dispersion).

Figure 5.11 - Schematic influence of dispersion on radionuclide concentration

Other transport processes (sorption and diffusion into the rock matrix) can retard the migration of radionuclides relative to the flow of groundwater (Figure 5.12). Considerable attention has therefore been focussed on understanding these processes and their affect on geosphere performance. Similarly, processes such as ion exclusion, colloid formation and surface diffusion can result in more rapid movement of radionuclides. Information on these transport processes can be obtained from both the field and in the laboratory and this is an area in which natural analogues can play an important role. Much of the available information on these processes is therefore generic and establishes that some are more significant in certain geological environments. Nirex research on these processes has been mainly in relation to their relevance to Sellafield.

5.3.1 Sorption in the geosphere

Sorption is an important mechanism for retarding radioelement migration from an underground waste repository (Figure 5.12). Nirex has carried out studies of the sorption of radioelements onto components of various rock formations that could be found in the geosphere [72]. These studies have focused on the generation of experimental data that can be used to quantify sorption (for use in assessments of the long-term performance of a
repository). Geochemical models of the sorption process have been developed to aid in interpretation of experimental data, and to allow limited extrapolation to conditions where direct experimental data are unavailable.

Figure 5.12 - Radionuclide retention processes
Minor iron and manganese oxides (present in most rocks) are normally considered to dominate sorption. The earliest Nirex studies of sorption onto rock samples (London Clay, Caithness Flagstones and St Bees Sandstone) [51] used ferric oxyhydroxide and goethite data to parameterise the sorption models. These models could reproduce many experimental trends, but problems were encountered when modelling data obtained under alkaline conditions [72]. It was recognised that minerals other than iron oxides could also contribute to sorption and so the sorption behaviour of other mineral types (other oxides, carbonates and sheet silicates) has been reviewed [106]. Sheet silicates such as chlorite and muscovite were identified as important alternative minerals with a capacity to sorb actinides significantly. A ‘two-site’ model was developed to represent sorption onto the aluminol and silanol sites exposed on the surface of these minerals [107]. In all the models, the main sorption mechanism was assumed to be surface complexation. Most of the radioelements studied tend to form negatively-charged or neutral species in solution and thus are unlikely to participate in ion exchange reactions.

The most widespread iron oxide mineral identified at Sellafield was hematite. Considerable effort has been expended by Nirex in the parameterisation of a robust mechanistic model of interactions of hematite with groundwater ions and aqueous radioelements [72]. A comprehensive dataset has been compiled including stability constants for surface complexation reactions for a range of univalent and divalent groundwater ions, and the radioelements selenium (IV and VI), uranium (VI) and plutonium (IV).

Iron oxide models were found to perform poorly when modelling sorption under alkaline conditions. Alkaline water-rock interaction results in the formation of secondary phases such as calcium silicate hydrates (CSH phases). It is believed that these phases dominate sorption under alkaline conditions. CSH phases are important components of cement, and so a model of sorption has been adopted based on the near-field cement model [108] (developed to represent sorption within the cementitious environment of a repository). This model has been used successfully to interpret results obtained under alkaline conditions.

5.3.2 Rock-matrix diffusion

Rock-matrix diffusion is the diffusion of radionuclides into pore space containing groundwater that is relatively immobile, such as “dead end” pores (Figure 5.12). Although these pores do not contribute significantly to the overall flow of groundwater though the geosphere, radionuclides can diffuse into them. Rock matrix diffusion effectively increases the total pore space accessed by the radionuclides and therefore decreases the rate of radionuclide migration relative to the groundwater. It is a radionuclide retardation mechanism identified principally for fractured rocks.

An extensive research programme by Nirex to investigate rock matrix diffusion parameters in a number of rock types [109, 58] has established an extensive database of the following properties:

- diffusion coefficients;
- porosity, measured by a range of techniques;
- hydraulic conductivity;
- rock matrix permeability;
- pore dimensions (including tortuosity) and
- surface area.
A methodology for determining these parameters in low permeability, low porosity rock matrices has been successfully developed by Nirex. In addition, natural analogue data demonstrate that, for uranium, diffusion distances of a few centimetres from fracture surfaces may occur in rock types such as granite. Measurements of chloride diffusion in granites adjacent to the Gulf of Finland has demonstrated diffusion on a scale of metres over a timescale of 5000 years. For uranium, these distances are significantly shorter than those often calculated for low permeability rocks in performance assessments. This may be because performance assessments tend to assume that uranium exists in the geosphere in the U(VI) oxidation state: this is a generally conservative assumption since, in this state, uranium exhibits weaker sorption and this allows faster migration of the uranium. As a consequence of this the calculated diffusion distances will be overestimated (since uranium migration is being modelled as less retarded than occurs in nature). An alternative explanation is that laboratory experiments overestimate diffusion coefficients because of the de-stressing and possible micro-fracturing that take place when the rock is removed from depth. While diffusion measurements on in situ granite have indicated that this is not the case, this finding needs to be confirmed for other rock types.

5.3.3 Colloids

Groundwater colloid populations are by nature site-specific and a safety assessment for any potential repository should address the potential impact of colloids based on site-specific colloid data. However, the study of colloidal transport of radionuclides in the geosphere by Nirex has addressed both generic and site-specific aspects of colloid behaviour with work concentrated into five main areas as follows:

- site-specific colloid studies including the development of sampling methodologies and subsequent characterisation of colloid populations;
- the distributions of natural uranium series isotopes between colloids and in solution in groundwaters;
- laboratory-based studies of colloid stability and surface properties using model and site-specific materials;
- colloid transport through geological materials including laboratory based studies of transport through natural fractures and field experiments in a fractured rock; and
- interpretative modelling of laboratory migration data using simple models of colloid transport and retardation.

Since 1991, Nirex geosphere colloid studies have focused on the presence, stability and mobility of colloids in the groundwaters at Sellafield. Owing to the low oxidation potential of groundwaters from Sellafield, a key aspect of the colloid characterisation work has been the development of colloid sampling methodologies that avoid oxidation of solutes in the groundwater sample (which can lead to the precipitation of iron compounds). Confidence in the ability to discriminate colloidal artefacts (i.e. precipitated iron compounds) from genuine groundwater colloids in reducing groundwaters is improving, and methods for achieving this continue to evolve.

Laboratory studies using synthetic silica and hematite colloids have played an important part in developing the understanding of colloid stability in groundwaters and mobility through fractured rock. The surface properties of synthetic colloids do not always represent site-specific materials well, however. Natural colloid populations are heterogeneous and it has been found that the sorption of low (ppm) concentrations of humic acid can modify surface potentials and influence colloid stability and migration behaviour.
Laboratory and field studies of the transport of synthetic silica colloids and naturally occurring colloids derived from fracture infill material have shown that colloids are mobile through geological media on length scales up to 15m. Therefore, colloids are potentially mobile in the geosphere [72]. However, these experiments have been performed at much higher flow rates than are typical of deep groundwaters. Reduced flow rate and increased ionic strength were found to favour increased colloid removal by attachment onto the rock surfaces [72].

A simple empirical model for colloid transport in fractures that accounts for reversible colloid sorption onto the fracture walls was able to successfully represent colloid transport behaviour in laboratory experiments [113]. Further testing of the model against data from different types of experiment under varying conditions is in progress to develop and build confidence in the approach and in the upscaling of the model to model colloid transport over length and timescales appropriate to performance assessment.

Some post-closure performance assessment calculations e.g. [12] have estimated the potential impact of colloids on radionuclide transport. At colloid concentrations that are typical of groundwaters in fractured rock environments, colloids in the geosphere have a negligible impact on calculated risk when radionuclide interactions with colloids are assumed to be reversible. However, the possible significance of irreversible sorption processes to colloids remains uncertain. In this case the risk will depend on the mobility and transport properties of colloids through the geosphere and the timescale over which individual particles remain in suspension.

5.4 Protection of the engineered barrier system

The development of repository proposals based on the multibarrier containment principle assumes that the various barriers are complementary. One of the functions of the geosphere is to provide a certain amount of protection to the engineered barrier system (see Section 5.1). Chemical compatibility between the geosphere and the engineered barrier system is one means of achieving a measure of protection.

In addition, the geosphere protects the engineered barrier system from future human actions (human intrusion) or from various disruptive natural events and processes. The likelihood of such intrusive or disruptive events and processes occurring will be in part dependent on the properties of the geosphere.

5.4.1 Chemical Compatibility

The long-term stability of all engineered barrier systems is closely related to the surrounding groundwater chemistry. Chemical conditions at depth that maintain the longevity of the engineered barriers are therefore desirable attributes. However, the conditions that provide this environment will vary for different engineered barrier systems. In very general terms, reducing conditions will support the development of reducing conditions in the engineered barriers as the cementitious barriers degrade. In addition, the evolution of the hydrochemical system at depth at potential repository site should be slow, so that the future behaviour of the engineered barrier system and its interactions with the geosphere can be modelled with confidence. To achieve this, the deep groundwater system needs to be relatively unresponsive to external changes and this can generally be achieved if hydraulic conductivity and/or hydraulic head gradients are low.
5.4.2 Human Intrusion

Human intrusion encompasses a range of human activities that have the potential to disrupt or impair the containment properties of the engineered system or the geosphere [114]. Human intrusion could be intentional or inadvertent. Intentional human intrusion, that is deliberate intrusion into the repository in the knowledge that it contains radioactive materials, is generally considered to be the responsibility of the society taking the action. Inadvertent actions are those where the repository or part of its barrier system are accidentally penetrated because knowledge of the repository location has been lost or its purpose forgotten. Possible inadvertent acts of human intrusion include drilling into the repository or the surrounding rocks, the excavation of material and the exploitation of resources such as water. Clearly, such actions could affect the long-term performance of the engineering barriers (and, possibly, the geosphere barrier also) and have direct radiological consequences for those involved in the intrusion activities.

The nature of human intrusion and the likelihood of its occurring will be dependent on the properties of the geosphere [8]. For instance, underground exploration will occur primarily in areas considered to have potential to provide an economic resource (coal, oil, gas, minerals etc.). Thus the risk of intrusion for candidate sites can be evaluated by consideration of their resource potential.

5.4.3 Natural Disruptive Events and Processes

Natural events that could disrupt a repository include earthquakes, meteorite impact and volcanism. The British Isles are located in an intraplate setting and as such they are expected to be subject generally to low levels of seismicity. Historically, small or moderate earthquakes of up to magnitude 5.5 have been registered [115]. Infrequent earthquakes exceeding magnitude 6.0 do occur in intraplate settings and some of these may be associated with the loading and unloading of ice. Other natural disruptive events such as meteorite impact and volcanism have very low probabilities of occurrence in the United Kingdom.

Natural processes that could disrupt a repository (e.g. erosion, ice sheet advance and retreat, sea level rise/fall) are mostly associated with climate change (erosion being highest at the extremes of climate). The most likely future climatic evolution of the UK involves continued glacial-interglacial cycling [116] and it is therefore likely that the nature and rates of erosive processes will be similar to those that have operated at different rates and for different periods throughout the Quaternary. Erosion depths due to downcutting by rivers are typically no more than a few tens of metres over a glacial cycle. Downcutting rates in limestone (likely to erode relatively quickly in these circumstances) of 2 - 5m in 105 years have been suggested [117]. However, the erosion effects of glacial activity are more uncertain. Nirex has developed a multidisciplinary approach to the study of the Quaternary period that has been successfully applied at the Sellafield site [118]. Such an approach could be equally applied at a different potential repository site at a suitable stage in the repository development programme.

5.5 Gas migration through the geosphere

The geosphere has a significant role to play in the gas pathway since the properties of the geosphere will control the way in which any gases generated in a repository will migrate to the surface. There are two mechanisms by which gas generated within the engineered repository can migrate back to the surface: either in solution in groundwater or as a separate gas phase [119]. In the latter case, the gas may move as bubbles or as a continuous gas stream. Gas phase migration as bubbles will be driven by buoyancy forces, in which case
movement will be predominantly vertical. For gas phase migration as a continuous stream, movement is driven by the gas pressure and there is the potential for lateral migration.

The relative magnitudes of the contributions of the different mechanisms will depend on the gas generation rate and the properties and state of the rocks through which the gas is passing. In general terms, gas migration through the geosphere could potentially:

- reduce the chances that gas over-pressurisation will exceed acceptable levels within the repository;
- accelerate the migration of radionuclides dissolved in groundwater by, for example, entrainment of water in a stream of gas bubbles, pressure induced groundwater flow, and the creation of unstable two-phase flow that could allow contaminated water to move closer to the surface by re-entering channels that were previously gas filled;
- carry additional radioactive material in the gas phase to the surface (for example naturally occurring radon); and
- cause a flammability hazard.

Gas migration modelling is generally carried out to determine whether gas can escape from the engineered repository and from the geosphere without deleterious effects on repository performance and to determine the nature of any gaseous releases at surface (including the degree of localisation) to allow the potential radiological impact or flammability hazard of the gas to be assessed. A number of different modelling approaches (Figure 5.13) have been developed that include simple scoping studies and more detailed numerical simulation. Nirex has developed capabilities in gas modelling using the program techSIM [120] that supersedes a previous gas program PORES [121].

This subject has also been considered in the light of evidence from natural analogues, principally seepage of petroleum-derived gases [122]. This work shows that gas seepage from deep petroleum wells is frequent, suggesting that repository over-pressurisation is very unlikely. This study notes that ‘with regard to modelling, successful predictions within the hydrocarbon exploration industry depend very much on the quantity and quality of subsurface geological data. Given the depths at which hydrocarbon accumulations develop, typically below 1000 m, such data are relatively limited. Generally, the lack of quantitative data on flow/flux rates reflects the primary objectives within the petroleum industry for which most investigations have been carried out: either to help identify potential petroleum reservoirs, or even more basically, to determine the origin of gases observed at the surface’. This work reinforces the view that the numerical simulation of gas migration from a repository will be very site-specific. It is likely that the petroleum industry will become a useful source of natural analogue information in future years. If so, this may add a another line of evidence to reinforce the numerical simulations.

The principal data required to carry out a numerical simulation of gas migration from a repository are:

- the fluid properties of the gas and water phases; that is, viscosity, density and compressibility and the solubility of gas in water;
- the geological structure of the host rock and the rocks between the repository and the surface;
- rock properties such as porosity and permeability, together with their spatial distribution;
• relative permeability and capillary pressure as functions of gas saturation (these two properties characterise two-phase flow through the rocks);
• gas generation rates within the repository; and
• the repository design and the physical and chemical properties of the materials within the repository.

**Figure 5.13 - The relationship between the programs used to assess potentially significant gas processes**
The ease with which these data can be obtained varies. Fluid properties are easily accessible and the geological and rock properties can in principle be established during the investigation of a particular site. The physical and chemical properties of the materials within the repository are affected by design and can be bounded. The data that are the most difficult to obtain are the relative permeability and capillary pressure functions of low permeability host rocks, especially if those rocks are fractured.

Significant work has been undertaken by Nirex to develop methods of providing and simulating these data in order to assess the effects of gas migration [73]. Crucial to the confidence in an assessment of gas migration is the application of a validation process to the gas migration models. A variety of gas migration experiments have been undertaken by Nirex at a research site in a disused slate quarry at Reskageage Farm in Cornwall. The methods used for validation at this [123] fracture rock site could be transferred to a specific site under investigation as a potential location for a radioactive waste repository.

5.6 Site characterisation issues

The performance of the geosphere barrier will be very dependent on the properties of the site under investigation. The ability to characterise these properties at a site is therefore key to the science underpinning a repository development programme [124]. In general terms, the role of site characterisation in supporting the development of repository proposals is understood. In consequence, the information and data required from a site investigation programme can be identified in a broad brush manner. The approach to site characterisation needs to be sufficiently flexible to adapt and develop as information about the site becomes available.

As the characterisation of a site progresses to support different stages of the siting process, the amount and detail of information required, and the range of techniques used to generate the necessary information increases. There is typically a gradual transition in investigation techniques which can be seen in many programmes. Initial desk studies of existing information generally precede remote sensing, geophysical surveys and geological mapping applied over successively smaller study areas in greater detail. Borehole drilling permits the \textit{in situ} testing, sampling and analysis of the rock mass (Figure 5.14) and groundwater body.

The construction and development of underground laboratories, permitting access to large volumes of the geological formations under consideration, is generally considered to be an important component of the site confirmation stage.

The design and implementation of a site characterisation programme, depends on:

- the type of geological environment being investigated;
- the repository concept; and
- the stage of the repository development process (see Figure 3.3) and the nature of the decisions required at each stage.

For example, different tools and techniques will be more or less appropriate in different environments and the amount and detail of information required generally increases as the siting process develops. It is therefore inappropriate to seek to prescribe an approach to site characterisation that is applicable generically. The following sections discuss the approach to site characterisation (in particular, aims and strategic principles) in general terms, and then discuss in more detail some specific issues relating to surface and underground based investigation techniques in different rock types.
5.6.1 **Approach to site characterisation**

Site characterisation programmes are required to provide information to:

- understand the performance of the geosphere at a potential repository site;
- demonstrate a broad based, self consistent geological understanding of a site (this includes geology, hydrogeology, geotechnical aspects and the geochemistry of the site) to a wide audience;
- develop practical engineering designs for the construction of a potential repository; and
- enhance the generic understanding of key processes that will impact geosphere performance;
- understand the potential interactions between engineered barriers and the geosphere over long timescales; and
- develop an assessment of the post-closure performance of a potential repository.

The broad types of information required from a site characterisation programme are therefore:

- structural and lithological information on the disposition, internal structure and inter-relationships of all of the rock formations in and around a site, to depths below the potential repository location and including surface sediment cover and soil formations;
- distribution of hydraulic properties of each formation, in terms of permeability, porosity, and nature of groundwater flow through rock units and individual structural features and the connectivity of different features in which flow occurs;
• geochemistry of rocks and groundwaters in different formations and features (e.g. faults and fractures), including hydrochemistry, fracture and pore surface mineralogy and chemical indicators of groundwater residence times and movement;

• information on the spatial variability of all the above properties and on the spatial scales over which they can confidently be interpolated or extrapolated;

• indicators of the potential variability of these properties with time;

• conceptual models of groundwater flow under current conditions and indications of how this could change in the future;

• indicators of stability or instability of the geological or hydrogeological system from the geological record, including evidence for recent (neotectonic) structural movements or environmental changes;

• indications of the resource potential of the different rock units and evidence of past drilling and excavation practices; and

• in situ rock stress distributions and geomechanical properties within each formation and in major structural features.

Site characterisation programmes need to be able to evolve as information becomes available. Of primary importance is the ability to review information against the identified aims in order to establish how understanding is developing and where there are key remaining uncertainties. For this reason, iterations with the development of repository designs, performance assessments and with scientific peers and the public are required. The stepwise process of repository development (which facilitates public consultation at key stages, Figure 3.3), the iterative repository design process and assessment cycles (Figure 3.2) provide a good framework for managing these iterations. It is therefore important that a site characterisation programme is sufficiently flexible to adapt and refocus, based on the outcome of these iterations.

A number of activities are linked in the process of site characterisation. These are identified in Figure 5.15. The manner in which they are linked is often complex and changeable. If the site characterisation programme is to be flexible and evolve in line with the overall repository development programme, the process of site characterisation is not a simple sequence of activities.

Planning is a very important aspect of any site characterisation programme. The purpose of each phase of investigations must be established and the relevant techniques identified, taking into account any practical constraints. Raw (or primary) data can then be generated by measurements in the field or on samples analysed in the laboratory. This primary dataset may require processing, either because the primary data are not directly representative of the in situ conditions (gaining access to the sample can disturb the natural environment) or because the measurement is correlated in some way to the data of interest. Data processing gives rise to a secondary dataset (processed data). The information of most relevance in establishing the characteristics of a site is often derived from the secondary data by interpretation. For example, models of the geological structure are extrapolated from information from boreholes and from geophysical surveys. Groundwater compositions are often compared by examining the ratios of certain chemical species. Finally, integration of many data from many different sources can provide a more comprehensive understanding and can help to reduce uncertainties arising from a single dataset. It can also provide an independent verification of conclusions drawn from any single dataset, thereby increasing the self consistency and confidence in conclusions drawn from independent data.
Establishing when enough information has been collected from a site characterisation programme is challenging. This can be facilitated if the programme is designed with clear aims, and by testing available information against those aims at various stages by the iterative processes described above. However, there will inevitably be limitations in the information that can be obtained from site investigations. These limitations may be imposed by practical constraints (for example never having complete coverage of information, limits of detection for different measurement techniques), by safety considerations (not destroying the beneficial properties of the site by the investigation process), or by judgements that the cost of obtaining the potential information is not consistent with the added value that it could provide.
The calibration of groundwater flow models is an important part of the investigations of a site. Nirex 97 [12] provides a detailed account of how this calibration was carried out for the Sellafield site, by using groundwater temperature, salinity and groundwater pressure data, together with the constraints applied by other attributes of the geochemical system. These were steady-state groundwater flow models and it is known that, in common with probably all potential deep disposal sites, the hydrogeological system of the Sellafield area is still responding to past changes, such as changes in sea level and ice loading. Nevertheless, the models developed were shown to provide an acceptable representation of the observable hydrogeological conditions in terms of groundwater head, salinity and temperature.

Box 5.1 - Characterising strong fractured (e.g. crystalline) rock exposed at surface

Experience from Sweden and Finland suggests that a characterisation programme where fractured rock is exposed at the surface is likely to be easier in some respects than one in a sedimentary environment where the host rock is not exposed. In particular, characterising a strong rock is likely to have the following advantages:

- Surface exposure of the rock allows significant areas of the rock mass to be examined at an early stage of the programme - although this is very dependent on the extent of exposure, which could be very limited. Where exposure is limited, as is commonly the case in inland areas of Finland for example, it may be relatively easy to examine the rock mass by digging investigation trenches.

- The drilling of boreholes in strong rock is less likely to require mechanical stabilisation through the use of thick drilling muds and/or steel borehole casing, both of which could hinder the collection of representative groundwater samples. In such cases groundwater samples may only be obtained during the underground RCF-phase of the investigations.

On the other hand, seismic techniques are generally less applicable to strong (e.g. crystalline) than to sedimentary environments, although seismic surveys have played a role in existing investigations in Sweden and Finland and are planned in future characterisation programmes [125].

5.6.2 The effect of geological environment on site characterisation

A site that is highly geologically complex will be more difficult to characterise than a less complex site [126]. A current challenge is that of confidently translating complex site characterisation information into tractable models which, despite their simplifications, provide an adequate description of site behaviour. Some types of site are more amenable to such simplification than others and the extent to which a simplified model can be developed will affect the amount and density of data needed to condition and test it. This has been described using the term the ‘explorability’ of a site [126]. The argument is that a robust assessment of a site is only thought to be possible if the site can be investigated.

In considering a potential setting for deep disposal a balance needs to be struck between:

- its ease of characterisation;
- the uncertainties that will be irresolvable after the site characterisation programme; and
- the likelihood of such an environment proving suitable with respect to long-term safety.

For example, it may be somewhat easier to investigate an environment where strong fractured rocks are present at the surface (Box 5.1); however it may be difficult to make a
convincing safety case for such an environment for the disposal of long-lived ILW [8]. Conversely, it may prove more difficult to characterise a sedimentary environment, or one in which sediments overlie basement rocks, but such an environment may offer a better prospect of delivering long-term safety.

The UK has a varied geology with a wide range of different rock types, both crystalline and sedimentary, with different hydrogeological properties. A repository site could be developed inland or by the coast. Topographical relief varies significantly across the country, from relatively flat plains to more mountainous areas. In consequence, there is a range of possible future disposal environments in the UK. These include the following:

- a strong fractured rock environment, exposed at surface i.e. similar to potential disposal environments in Scandinavia and Canada;
- a sedimentary sequence in an area of simple structure, where the repository host rock would be a low permeability argillaceous sediment, i.e. similar to the current Meuse/Marne underground research laboratory site in France; and
- an environment where the disposal facility is in a strong basement rock located under sedimentary cover as at Sellafield but where the sedimentary sequence is generally thinner than at Sellafield.

This list is not meant to be exhaustive and is also not intended to pre-empt any future site selection programme. The environments identified are similar to those represented by the illustrative groundwater flow models developed recently by Nirex [8]. Boxes 5.1, 5.2 and 5.3 discuss issues relating to the investigation of these three different types of environment.

Nirex has obtained considerable experience in carrying out site characterisation programmes. Much of the experience that Nirex has built up could be transferred to any of the known potential disposal environments. In addition, experience of site characterisation in a wide range of geological environments has been obtained in other programmes e.g. [101]. Disposal programmes in Switzerland, France or Japan, where a variety of disposal environments are present, will be highly relevant to any future UK investigations, as will those in Canada, Sweden or Finland, where only strong, fractured rocks are being considered.

Thus, whilst the style of the characterisation programme is likely to vary considerably between sites in different geological environments and the emphasis on the use of different techniques will also vary, the majority of techniques needed to obtain the necessary information exist.

For example, in strong fractured rocks it is possible to drill small diameter boreholes without the use of casing except near the surface. Such boreholes provide good access to the rock mass and can easily be inclined or deviated. Small diameter wireline logging tools, hydraulic testing and geochemical equipment has been developed, particularly in Sweden and Finland, to allow an extensive site characterisation programme to take place. In sedimentary rocks, however, particularly ones with weaker argillaceous sedimentary formations, casing is likely to be needed for borehole support. However, the application of techniques to the characterisation of sedimentary formations is well supported by the development of tools for the oil industry.

The measurement of chemical attributes of groundwater in boreholes is difficult and, depending on the rock type and the accuracy that is considered necessary, may not be possible until access is provided to the rock at depth from an underground characterisation
Box 5.2 - Characterising a sedimentary environment

There is less international experience of site characterisation for radioactive waste disposal in deep sedimentary disposal environments, as only recently have investigations in such environments been conducted in France and Switzerland (at the Gard and Meuse/Marne prospective underground research laboratory sites in France and at the Opalinus Clay borehole at Benken in Switzerland). The Mol site in Belgium, where the underground research laboratory is at a depth of 220 m in plastic clay, is somewhat atypical of potential sedimentary disposal environments that have been considered in other countries. The operating repository at the WIPP site in the US has been constructed within a salt formation, for which there is no analogy within the UK for the volume of wastes that need to be considered for disposal. There are, however, very extensive investigations carried out in such rocks for other purposes, in particular oil exploration. Over the last decade there has been an increased interest in the hydrocarbon industry in the lower permeability components of the geological succession, because of the need to consider the barriers they provide to oil migration.

Site characterisation programmes in sedimentary environments are likely to be considerably different from those in strong fractured rocks. Boreholes are likely to be required to similar depths but they will need to drilled and completed in a similar manner to the deep boreholes at Sellafield. Boreholes in some well indurated sediments may be stable without significant permanent casing and may allow the installation of multi-packer monitoring systems similar to those that were installed at Sellafield. Examples of such sediments are the Opalinus Clay in the Benken borehole in Switzerland and the Lower Lias sediments that were investigated by Nirex at Fulbeck. Similar sediments are present under considerable parts of eastern England. Seismic techniques, including 3D seismics, are more useful in this type of environment. Perhaps the main differences between these disposal environments are related to:

- the potential for reduced significance that is likely to be attached to fracture-dominated flow and transport in sediments. However, the significance of fractures and faults cannot automatically be discounted, in particular for argillaceous sediments at depth in the UK, which are likely to be well indurated, not soft clay formations.
- the greater problems that exist in sedimentary environments in the derivation of hydraulic properties from in situ measurements (due to the complex coupling of physico-chemical processes)
- the problems that exist in obtaining representative groundwater samples at depth in boreholes from the poorly permeable components of the succession, in particular in soft clay formations. This is due to the type of boreholes that are required combined with the low hydraulic conductivity of these rocks.

Whilst soft clay environments have been selected because they are believed to be associated with slowly evolving geochemical conditions and low groundwater flow velocities, it is precisely these attributes of the environment that make measurements in these rocks more difficult [127]. It seems likely that even more emphasis should be placed on hydrochemistry in these types of rocks than is the case for strong (e.g. crystalline) rocks, as the determination of their hydraulic conductivity is fraught with difficulties and the values obtained are subject to large uncertainties.
facility. One of the conclusions of Nirex’s investigations at Sellafield [128] was that the pH, alkalinity, Eh and colloid ranges measured directly in groundwater samples from deep boreholes in that environment were not reliable indicators of in situ conditions. Wide diameter oil industry drilling technology was used and heavy fluids were added to the borehole during drilling in order to provide the necessary stability and they affected the groundwater chemistry. However, through the addition of conservative tracers to the borehole drilling fluids and detailed data analysis and processing, good estimates of in situ groundwater compositions were obtained for most chemical constituents [129]. However, the reactive constituents Eh and pH were irreversibly affected by the drilling fluids and so in situ levels were not accurately determined from the borehole drilling programme. Instead, these levels were calculated by modelling the overall chemical composition of the groundwater.

**Box 5.3 - Characterising basement under cover**

Sedimentary rocks that overlie basement can, in theory, provide a dual groundwater flow system in which the flow can take place predominantly in the sediments and possibly in the upper parts of the basement, which may have an enhanced permeability. This is the case where there is little relief and where at least some of the sediments have greater permeability than the basement rocks. This was originally presented as a disposal concept by Bredehoeft & Maini [124]. Dilution and dispersion of any releases from a repository are likely to be advantageous and this subject is discussed in Kristallin-1 [101] and in [131]. Where the sedimentary rocks have a low permeability then they will tend to seal the basement rocks and, where no faults cut the sedimentary units, they are likely to provide all the advantages associated with low permeability sedimentary rocks (i.e. slow radionuclide transport rates), together with the advantages of a repository in strong rocks (i.e. ease of construction for large volumes of ILW).

A disposal environment in which a repository in located in strong basement rocks overlain by low permeability sediments of limited thickness may have advantages in terms of its long-term safety and ease of construction but, in terms of site characterisation, it may suffer from disadvantages, such as those highlighted and addressed by the investigations of such an environment near Sellafield and at Vienne. In general, the possible disadvantages are:

- the host rocks may not be visible, except in boreholes;
- the overlying sediments have low permeability, they could be difficult to characterise for precisely this reason (this is currently a problem in testing in the Benken borehole in Switzerland);
- the size of the investigation area could be large if hydraulic gradients are low (though this is preferable in terms of long-term safety), if an alternating sequence of high and low permeability sediments are present and if there are few faults;
- the boreholes will need to be designed to accommodate possibly weak sedimentary rocks. Borehole designed in such a manner can place limitations on the acquisition of certain data, in particular some chemical data; and
- the internal structure of the basement may be difficult to assess, since it is less likely to be exposed locally and is less likely be amenable to investigation using surface seismic surveys than a sedimentary rock, resulting in more restrictive and costly inter-borehole surveys being required.
In contrast, boreholes drilled by Posiva (Finland) were of small diameter and only surface casing was used. Posiva found that the borehole measurements of these parameters were reliable indicators of *in situ* conditions during their site characterisation programmes in strong, fractured rocks at four sites in Finland.

Large parts of the UK are covered with unconsolidated Quaternary deposits. The Anglian glaciation, more than 400 000 years ago deposited extensive glacial sediments almost as far south as London and subsequent glaciations have resulted in further glacial sediments being deposited in areas further north. These deposits can be several tens of metres thick and they blanket many lowland areas, predominantly with glacial till. In areas where there is minimal or thin glacial or recent cover it is possible to obtain direct access to the rock by, for example, digging inspection trenches or removing the superficial material from larger areas of the rock mass using high pressure water jets. Both of these techniques have been applied in crystalline rock areas in Canada, Sweden and Finland in areas where exposure was poor. Where such cover is thicker, however, it is not possible to do this and additional challenges emerge, such as the difficulty of carrying out seismic surveys in regions of thick cover, due to the attenuation of the seismic signal.

Where the potential host rock is overlain by other rocks, the characterisation becomes more difficult, and good examples of this situation are provided by the Nirex investigations at Sellafield, by the Nagra investigation area in northern Switzerland and by the Vienne site in France [130]. In all these cases the volcanic or granitic basement host rock, is overlain by considerable thicknesses of other rocks. Data on the characteristics of the host rocks could be obtained either from deep boreholes, which are limited in number, or from surface mapping in areas often distant from the site, where the host rock outcropped. For example, the conceptual model of major (water-conducting) fracture zones in northern Switzerland used information on the exposed area of such zones in the Black Forest of southern Germany [131]. Similarly at Sellafield, the Borrowdale Volcanic Group basement rock is exposed several kilometres to the east of the PRZ, where it has been mapped [132]. In addition, not being able to view the rock mass over large areas, its structure was determined using deep boreholes and cross-hole techniques.

There are difficulties associated with making measurements in soft argillaceous rocks due to the complex, coupled thermo-hydro-mechanical and chemical processes that control their behaviour. These are caused by the high surface area of the clay minerals. This subject has been thoroughly reviewed recently by Horsemann et al [133]. An increased level of understanding of these processes is being developed by *in situ* tests that are currently being carried out in the Opalinus Clay in the Mont Terri underground research laboratory in Switzerland.

Taking the various international programmes into account, site characterisation techniques are available for the determination of most properties in most rocks. The applicability of techniques and the uncertainties on measurements will vary for different environments. There are two areas where techniques have yet to be developed:

- the *in situ* hydraulic testing and measurement of solute transport in soft argillaceous formations (clays); and

- groundwater sampling techniques and down-hole *in situ* measurement techniques for reactive chemical constituents (in particular Eh and pH) in deep boreholes drilled into or through unstable formations.
5.6.3 Going Underground: characterisation from beneath the surface

It is internationally accepted that a phase of underground site investigations is likely to be required in order to characterise a site sufficiently to support a repository development programme. In the UK, the term Rock Characterisation Facility (RCF) has been used to describe a system of underground shafts and galleries in which such work would be carried out. All deep waste disposal programmes, e.g. those in France, Switzerland, Sweden, Finland, Japan, Canada and the USA, assume such a phase. Nirex has explained its rationale for having an RCF at Sellafield [134] and similar scientific arguments would apply equally for other disposal environments should they be selected in the future.

It has been acknowledged by both the DETR [135] and the House of Lords [18] reviews that a generic underground research laboratory (i.e. not at a repository site) would not be needed in the United Kingdom unless an unusual environment were being pursued by the site selection programme.

In considering the RCF stage of site investigations, it is appropriate to consider whether suitable equipment exists to carry out the necessary in situ tests. A large amount of sophisticated equipment has been developed over the last twenty years in the radioactive waste disposal field specifically related to in situ experimentation in underground research laboratories. Probably the greatest number of experiments have taken place in salt, at Asse, WIPP and associated with the now-abandoned US disposal programme for spent fuel disposal in salt, although a large number have also taken place in strong fractured rock in Sweden, Switzerland and Canada. It seems likely that no further, specific equipment requirements exist in this area.

Figure 5.16 - Mol underground research laboratory (with permission of SCK-CEN)

Experimental programmes in argillaceous rocks have recently become increasingly innovative. The experimental programme at Mol has been running for many years (Figure 5.16) and has formed a firm basis for the more recent experiments in the Mont Terri tunnel in Switzerland, where a new experimental gallery has recently been constructed. The research and development programme at Tournemire has also investigated the coupled processes that are such a feature of testing and experimentation in clays. In France plans are well advanced to have at least one underground research laboratory in a clay over the next
few years. The currently selected site, at Meuse/Marne lies in Jurassic clays that are similar to equivalent clays existing in the east of England. Equipment development is required in order to allow the necessary data to be collected from both fractured and unfractured argillaceous rocks.

Much of the emphasis of underground research laboratory work, especially in Europe but also in Canada, has been directed towards strong fractured rock. This has been due to the presence of internationally-based R&D programmes at Stripa and Åspö in Sweden, and at Grimsel in Switzerland.

Equipment development is continuing at Åspö and further experiments are proposed at Grimsel. There would appear to be only one area where new techniques might have to be applied and this is in trying to determine the flow-wetted surface area or reactive surface area of fractures and the role of fracture infill materials. This is an important attribute of the fracture system in determining the rate of radionuclide transport, and work is continuing to define how it could be measured. This subject has been discussed extensively by SKI [102] in terms of the retention mechanisms in strong fractured rocks.

The construction of an RCF or other underground facility will perturb the natural system and, in particular, the groundwater regime. It is necessary to have achieved an adequate understanding of the natural system in advance of any construction, because the changes due to construction will be irreversible. The construction of the facility also provides an opportunity to develop and test models of the site over large volumes of the rock mass.

“Baseline” is the term generally applied to the conditions in a system, e.g. a groundwater system, prior to some form of induced perturbation. The undisturbed conditions incorporate the effects of natural features and processes which account for the spatial and/or temporal variability in the system prior to construction of an underground facility. Baseline conditions for groundwater pressures and hydrochemical conditions need to be established prior to the construction of the facility. Sufficient information needs to have been acquired so that:

- the disturbance created by the facility can be measured and used to test and develop models of the site; and
- there is a sufficient database on undisturbed conditions that the properties of the rock mass in the region of the proposed repository can be interpreted within the context of the regional groundwater flow and hydrochemical models.

Nirex installed a comprehensive monitoring network at Sellafield using multiple packer systems (generally Westbay MP55 ® strings) to isolate a number of discrete zones in selected boreholes and monitor groundwater pressures and temperatures with time and sample periodically to obtain groundwater for chemical analyses [26]. This network (the Long-Term Monitoring System) provided time-series groundwater pressure data with sampling intervals generally ranging from 2 to 30 minutes which were combined with the Environmental Pressure Measurements (EPM) that had been previously obtained in the deep boreholes during drilling (Figure 5.17). Hydrochemical data were used in a more qualitative way to support the groundwater flow modelling. For example, hydrochemical characteristics such as the chloride concentration, which are not significantly modified by geochemical reactions, were used to infer directions of groundwater flow. Other hydrochemical data were interpreted in terms of the evolution of the groundwater system and the geochemical processes which occur in the undisturbed system.

Nirex was able to demonstrate to an international review group [136] that baseline conditions had indeed been established at Sellafield. Further monitoring using the Long-
Term Monitoring System has subsequently demonstrated that little has changed over a period of a further two years [137].

Similar baseline conditions were determined at Äspö in advance of underground construction and it is generally accepted that it is possible to determine such conditions using existing equipment and techniques at strong rock sites and at sites where sediments overlie the basement. The techniques that would be used in less permeable argillaceous sequences are likely to be essentially similar, although the potential changes due to construction may well be of lower magnitude, be measurable over a smaller volume of the rock mass and the response time of the system may be longer. There is no reason to suppose that baseline conditions could not be determined in any potential disposal environment.

*Figure 5.17 - Length of records for the long-term monitoring system at Sellafield*
5.6.4 Characterisation for repository design and construction

The geological properties of the site will also affect repository design and construction. Nirex has considered the geotechnical aspects of repository design and presented preliminary designs for repositories in both strong and weak rocks in a preliminary environmental and radiological assessment [138]. A more site-specific design was developed for Sellafield [139]. In order to provide a detailed design for any site, site-specific geotechnical data are required and the collection of such data was an integral part of the site characterisation programme at Sellafield [140].

The design of a repository for any type of long-lived waste is similar to the design of several other major underground structures, although there are notable differences. These include:

- the factors of safety that are likely to be required, both during the operational phase and post-closure;
- thermal considerations;
- the consideration of the length of time for which rock excavations remain stable without additional support in the event that retrievability is required;
- the requirement to consider the design not only in terms of its operational safety (as would be the case for a conventional underground structure, such as a hydroelectric scheme) but also in terms of its performance post-closure; and
- the requirements for monitoring that are likely to be considerably in excess of anything required for other underground structures.

Construction in strong, fractured (e.g. crystalline) rock is a relatively standard procedure and preliminary repository designs can be developed using:

- a knowledge of the geological structure;
- the volume requirements for waste disposal;
- the classification of the geotechnical properties of the rock mass - this would be carried out using a rock mass classification system (there are two main systems in use in Europe, the Q-system and the RMR);
- measurement of the magnitude and orientation of the in situ stress; and
- geotechnical modelling software.

Conventional geotechnical practice has developed techniques for generating this information based on data obtained from boreholes and from other site characterisation techniques. The geotechnical programme followed at Sellafield applied these techniques and was intended to have been followed by further geotechnical work within the RCF [134], where the actual measurements of the disturbance caused by the construction could have been compared with those predicted from previous modelling based on borehole data. The techniques and procedures for obtaining this information therefore exist. Stress measurement in strong rocks, using a variety of techniques, is now relatively common practice and was used to develop a stress measurement programme at Sellafield [140].

Disposal in sedimentary rocks is most likely to take place in thick argillaceous sediments at several hundred metres depth, and sediments of current interest include the Meuse/Marine underground research laboratory site on the eastern margin of the Paris Basin, the Opalinus Clay in northern Switzerland and the generic sedimentary site considered in Nirex Report 71 [138, 141]. Disposal in such an environment would require a very different type of
repository design which would most likely consist of a series of fully-lined parallel tunnels in which the lining may have to support the lithostatic load and could, therefore, need to have a considerable thickness, especially in the weaker argillaceous rocks. The lower strength of these rocks, in addition to requiring the lining, is likely to limit the maximum depth at which such a repository could be constructed. Depending on the shear strength of the clay it may be possible to construct small diameter tunnels to depths of 800 m (This is the maximum anticipated depth, for example, for the disposal of HLW/SF in the Opalinus Clay in Switzerland in 2.5 m diameter tunnels. At the design depth of 650 m it is currently anticipated that these tunnels would require minimal support, although it is the intention to backfill them soon after waste emplacement). Consideration of larger openings (for the disposal of larger waste forms or desirable for operational and cost reasons), host rocks with shear strengths below that of the Opalinus Clay and any requirement for long-term stability (for example, if backfilling were to be delayed), could require a greater level of support or a reduction in depth from the surface. The Opalinus Clay has a low moisture content and a high shear strength for an argillaceous rock. Some of the clays and mudstones that might be considered in the UK for the disposal of long-lived waste (e.g. see those sedimentary rocks considered in [8], also those sedimentary rocks considered in [142]) may have lower shear strengths and would require shallower depths for disposal. Other aspects of waste management, such as retrievability, could place additional constraints in this area.

5.7 Summary of knowledge base and capabilities

There is a considerable depth of international expertise in evaluating potential repository sites, not only in terms of field activities, but also in terms of analysing and utilising site investigation data in performance assessment and design. The Nirex experience at Sellafield has played a strong part in building this international capability, taking its share of the development work in the particular environment of deeply buried basement rocks. As a consequence, the UK expertise meshes well with that available worldwide. However, consideration of any future UK site investigation should not exclude geological environments which have so far not been evaluated in detail in this country. As a result of the overlap of expertise and the commonality of international approaches to site investigation methodology, this should not a priori present a problem.

It is important to know how to develop appropriate conceptual models of site properties, how to reduce complex data sets into useable information for performance assessment and design, where to look for the most appropriate supporting information on which to demonstrate an understanding of a site and, finally, when to stop gathering data. Much of the Nirex experience at Sellafield has explored these key areas, and Nirex believes that the Nirex 97 performance assessment [12] illustrates significant progress in conceptual model development and the reduction of complexity to produce manageable bodies of information.

Experience of site characterisation programmes over the last few years at potential radioactive waste disposal and R&D sites has shown that the success of a site characterisation programme is not normally controlled by the availability of techniques. It is determined to a greater extent by the experience of the site characterisation team and the way in which the site characterisation programme is linked to the requirements of the performance assessment.

Nirex has developed considerable experience of investigating one type of disposal environment and much of this experience can be transferred, directly or indirectly, to the characterisation of other types of environment. It is likely that the emphasis placed on the various aspects of the site characterisation programme would need to be re-evaluated were
other types of environment to be investigated. However, such an investigation would not require much new equipment to be developed; any problems might relate more to the level of investigation necessary to gain sufficient understanding of these different environments to support a repository development programme.

Although the approach to deploying site characterisation techniques will vary from site to site (and from one geological environment to another), the field techniques themselves are already well-developed and essentially to hand. Two areas have been identified which will require substantial further technical development in the run-up to new site studies. These are (1) the sampling of chemically representative groundwaters and colloids from deep systems and (2) the measurement of representative in situ hydraulic and transport properties of deep argillaceous formations. If the siting programme were to focus on strong fractured rocks (for which there are advantages in the construction of large openings at depth for some categories of wastes) then the latter is not an issue.

The sampling of groundwaters for chemical analysis and interpretation is seen as a key area, because it is the basis of much of the palaeohydrogeological analysis which will support conceptual models of site evolution. Nirex has probed deeply into this matter, but will need to continue technical development work for environments other than strong fractured rocks exposed at the surface. Similarly, further work will be needed in the collation and interpretation of the range of information which makes up a palaeohydrogeological evaluation.

A phase of underground rock characterisation in an RCF-like facility is likely to be essential. The technical basis for working in an RCF is well developed internationally and ready for application in almost any environment that may be selected. Continued UK involvement in international underground research laboratory projects in the intervening years before any UK repository development programme might be started will help to maintain this capability until it is needed. Most parties are currently agreed that a UK generic underground research laboratory would be unjustified unless an unusual disposal environment were to be considered.

Underground construction will disturb a site considerably and it will be important to establish baseline conditions prior to disturbance. This baseline information will also form the foundation for a long-term environmental monitoring programme which could extend well beyond the time of repository closure. Nirex has developed an approach to defining key baseline conditions; this approach would be transferable to another site and could be incorporated into the earliest stages of planning a site investigation.
6 CHARACTERISING THE BIOSPHERE

In this chapter, the state of knowledge relating to the biosphere is summarised. The biosphere is defined on page 2.

6.1 The role of the biosphere

A robust safety case for the disposal of radioactive waste to a deep geological facility should demonstrate that the wastes would be contained and isolated for very long periods of time. Unlike the engineered barrier system and the geosphere, the biosphere is not generally considered as a barrier to radionuclide releases. Rather it is the receptor for such releases, where radionuclides may be either dispersed or accumulated. Radionuclide behaviour in the biosphere will determine the accessibility of radionuclides for uptake by humans, and the radiological dose that may be received as a result of this uptake [143].

The siting of a repository is normally based on the demonstration of a suitable geological environment since it is the characteristics of the host rock formations that will act to protect the engineered barrier system and to limit the transport of any radionuclides released from the repository (see Section 5). The biosphere environment in the vicinity of a repository is not usually a discriminating factor in site selection, because it is necessary to consider the type of biosphere into which radionuclides may emerge at some distant time in the future. At that point in time, the biosphere is likely to be different to that currently prevailing. As it is not possible to predict the nature of the future biosphere into which radionuclide release will occur, research is targeted at developing methods for the representation of a range of possible future biosphere systems [144]. This necessitates understanding the key processes that influence the biosphere over long time periods, how radionuclides might be transported into the surface environment and the factors that determine the behaviour of the radionuclides once present in the biosphere. Key issues in relation to the biosphere are therefore (Figure 6.1):

- the range of possible biospheres into which radionuclides from the repository could be discharged; and
- the behaviour of radionuclides once discharged into the biosphere.

6.2 The description of future biospheres

The evaluation of the transport and behaviour of radionuclides within the biosphere over long timescales into the future requires an understanding of the mechanisms that control biosphere change. With this understanding, relevant information on past and current biospheres can be used to provide the basis for representing future biospheres. There are three principal factors that influence the characteristics of the main components of the biosphere and that lead to changes in the environment. The first is climate-driven change; the second is landform change and the third is Man’s influence on the environment, anthropogenic modification. Assumptions are made that future society will operate in much the same way as today and in the past, with a broadly similar level of influence on the surface environment (e.g. with regard to agricultural practices). Consequently, (with the exception of the effects of greenhouse gas emissions) large and long-term changes are considered to be unlikely as a result of Man’s activities. The influence of mankind, as a control on biosphere evolution, is not considered further in this section.
6.2.1 Climate and Climate Change

Climate is the main controlling influence on many biosphere components including: soil type, animal and plant communities, and water body characteristics. It is therefore necessary to understand how climate and climate change act upon the biosphere to cause environmental change.

Climate changes in response to a wide variety of factors. The Earth’s general climate has fluctuated between cold and warm periods and between dry and wet conditions on a number of occasions during the last four and a half thousand million years. However, it is the pattern of climate change observed over the last two million years, the geological period known as the Quaternary, that can provide information on how climate might change in the next million or so years.

Climate studies have shown that the long-term global climate has undergone a number of glacial/interglacial cycles over the Quaternary. Statistical analysis of data from cores taken from ice sheets and deep sea sediments, together with isotopic analysis of fossilised organisms (benthic foraminifera) and other proxy indicators (Box 6.1), give insights into past climate and make it possible to reconstruct past climate sequences. The broken line in Figure 6.2 shows one such sequence [145]. Climate reconstructions show that the current temperate climate is representative of less than 15% of the past 400,000 years. The majority of the time (ca. 75%) has been boreal or periglacial, with the remainder glacial.
Box 6.1. Relevant information on past climates

Climate reconstructions of the last glacial/interglacial cycle have been carried out on the basis of a range of proxy indicators [154]. Techniques used by the various scientific groups involved in such work include: the physical and chemical analysis of ice cores e.g. [146, 147]; analysis of oxygen isotope ratios and organism remains in ocean cores [148, 149]; analysis of speleothems (stalactites, stalagmites and flowstones) [150]; consideration of palaeogeological data (e.g. coral reefs) [151]; and other non-marine geological and biological evidence such as pollen analysis. On behalf of Nirex, the Climate Research Unit (University of East Anglia) has provided a detailed review and analysis of the literature for development and decline of past climate states (i.e. Glacial, Tundra, Boreal, and Temperate climate states) and climate state sequences [152, 154, 155].

A considerable amount of work was carried out to characterise the sediments laid down during the Quaternary period in the vicinity of Sellafield [117]. The evolution of the sediments in this area during the Quaternary was complex due to its location at the coast of the shallow Irish sea and due to the influence of ice sheets derived from both the Scottish and Lake District centres.

The objectives of the Quaternary studies in the Sellafield area were primarily to (i) reconstruct the Quaternary geological history; (ii) provide background information for the near-surface hydrogeological work and (iii) describe the deformation structures in the Quaternary deposits and interpret them for evidence of the mechanisms causing such deformations. Whilst these investigations were mainly applied to the near-surface hydrogeological modelling work, they also provide an understanding of how past biospheres have evolved to produce the biosphere today. For example, core analysis of peat from Hallsenna Moor near Sellafield has provided a pollen record of the period following the post-Late Devensian Glaciation that has helped with palaeoenvironmental reconstruction. Hand augering and piston coring have also been used to study the history of various marine and estuarine deposits. This demonstrates that even for a relatively complex sediment history, techniques are now developed to provide the necessary understanding.

Frequency analysis of these sequences has shown cycles (periodicities) in long-term climate change, similar to those of changes in the Earth’s orbit around the Sun. On the basis of this orbital cycling, it is considered likely that up to ten more glacial/interglacial cycles will occur over the next million years. The link between such astronomical cycles and the long-term climate is known as the Milankovitch Theory. A vast body of literature has been produced on the nature and mechanisms of climate change. This information has been reviewed, summarised and published by Nirex based on the work of the Climate Research Unit at the University of East Anglia [152, 153].

Evidence for the mechanisms of short-term climate change, operating on timescales of a few thousand years, possibly down to decades, has also been studied [116]. Such short-term changes are due to natural mechanisms (such as solar variability, changes in wind and ocean currents and volcanic action) and, more recently, to human influences such as enhanced levels of so-called ‘greenhouse’ gases and sulphate aerosols. Work by Nirex and its contractors is ongoing with respect to modelling the consequences of human-induced climate change and the potential impacts this might have on the sequence of long-term climate change [154].
Figure 6.2 - Past climate and the Louvain la Neuve climate model

a) Global ice volumes simulated for the last 122 thousand years compared with reconstructed record. The model is forced by insolation only.

b) Global ice volumes simulated for the last 122 thousand years compared with reconstructed record. The model is forced by insolation and the Vostok CO2 record.

In both cases the reconstructed record is from LD Labeyrie et al, Nature, 327 (6122), 477-482, 1987 and the figure is based on A. Berger et al., Journal of Glaciology, 39 (131), 45-49, 1993.
There is therefore a large body of information regarding the processes and effects of climate and climate change. Much of this work has been reported by the Climatic Research Unit as part of the Nirex science programme [152, 153, 154, 155], in international workshops [116], general publications e.g. [156, 157] and scientific conferences e.g. [158, 159].

In addition, there is experience of addressing the effects of climate change on the biospheres as part of undertaking performance assessments. Many major repository performance assessments have involved an explicit consideration of the development of future climates, e.g. in Canada [160] and in the U.S.A. [161] and also through work on behalf of the UK regulators [162, 163]. Other performance assessments have, to date, implicitly incorporated the effects of alternative climate states (e.g. Nirex 97 [12]).

6.2.2 Landform Change

Closely, but not necessarily directly, linked to climate change is landform change and development. This association between climate and landform development exists because the Earth’s surface is constantly being moulded by the agents of change, such as wind, heat and precipitation in its various forms. In situ weathering, both mechanical and chemical, is accompanied by the transportation of detritus, leading to erosion and re-deposition. Glacial events result in major changes to the volume of water and ice present in the environment, and the movement of ice sheets and glaciers can cause appreciable surface topographical changes and alterations of sea level. On the basis of results from climate studies, geomorphological investigations are being used to define processes and rates of landform change in different climate states. Work has been completed on topics such as:

- the advance and retreat of ice sheets [164];
- glaciation in the British Isles [165];
- glacial and non-glacial erosion [166, 167]; and
- the various geomorphological process and rates which occur in periglacial (tundra) and boreal (subarctic forest) climate states [168, 169].

Initially, mainly qualitative information was collated on the above subjects. However, from 1992 onwards more quantitative studies have been undertaken. For example, evidence of landform change brought about by glaciation can be obtained from studies of the erosion of upland and lowland features and how rivers have become diverted over the course of time. The University of East Anglia and others have constructed a spatial database which covers most of Britain [170, 171]. This contains variables associated with the development and nature of regional-scale relief. Factors such as elevation, geology, river length and local variations in gravity have been recorded at a grid scale of 1 km² [172]. From this information, a digital relief map of Northern Britain has been developed in order to assist with the reconstruction of the historical pattern of erosion for selected areas. This is useful for modelling future patterns of erosion and relief in line with future climate change studies.

Quantitative models of ice sheet growth and decay are currently being developed. Since many interlinked processes are involved, model development is taking place in stages, with model intercomparison exercises being used to compare results [172]. The descriptive models of glacier/ice-sheet development and movement have been based on data collected from the Nirex programme to characterise the Quaternary in Cumbria [118].
There is general agreement on the broad pattern and timing of the build-up and decay of ice during the latest glacial phase, the Late Devensian glaciation, the extent of ice cover and the directions of ice movement. Figure 6.3 illustrates recent understanding. However, the future limits of ice sheet growth and decay and the exact timing of the ice advances and retreat are not well known. Whilst significant progress has been made with the understanding of the climate processes causing landform changes, an evaluation of the significance of ice sheets, in terms of its impact on and surface erosion, is a topic that will require a site-specific understanding as part of any future detailed site characterisation programme. (The effect of ice sheets on groundwater flow is discussed in Section 5). Clayton [166, 167] has summarised work on quantification of glacial erosion and denudation rates in the British Isles.

The presence of ice sheets, sediment deposition and the transgression of the sea onto a former land surface all have a loading effect on the earth’s crust. As an example of such an effect, the land surface of NW Britain was depressed by 200-300 metres under several hundred metres thickness of ice during the maximum phase of the last glaciation. Depression of the Earth’s surface due to such loading is followed by crustal rebound once the load is taken away, either due to the retreat of ice sheets, erosion or the regression of the sea. Based on the study of Quaternary sequences and geophysical data, some authors have postulated the presence of moving ‘forebulge’ effects, peripheral to the load, during ice sheet loading and advance [165]. If such an effect exists, it would result in the local elevation of the land surface in the area in front of the ice sheet, relative to a fixed datum. The dynamics of loading/unloading effects, in terms of rates and the degree of vertical uplift and subsidence, are governed by visco-elastic deformation of the asthenosphere, which underlies the earth’s crust, and by the degree and timing of loading. The surface of the Earth is always seeking to attain a state of dynamic equilibrium through the loading/unloading process described above, which is termed isostatic readjustment.

Another major effect of glacial/interglacial cycling is that sea level varies considerably over a glacial cycle. This is relevant to performance assessments because the position of the coast could decide whether radionuclide releases from a repository occur directly to sea or on land. The variation in global sea level could be over 25 metres above the present level during warm periods (Temperate or ‘greenhouse gas’ warmed), to 130 metres below present levels at times of maximum ice sheet extent [173]. The main cause for this change is the development and regression of continental ice sheets, which can incorporate a significant proportion of the total volume of global waters. Variations in local sea level can be different from those observed globally due to vertical (isostatic) movement of the land mass. The University of East Anglia and others have undertaken extensive reviews of the effects of climate change on global and UK sea-level changes on behalf of Nirex [152, 153, 154, 174] and models are available for assessing historical sea levels around Britain [175, 176].

Other landform changes that occur on time scales of 100 to 10,000 years relate to the development of rivers and soils. The courses that river systems follow are likely to change in the future, due to coeval incision (erosion) and/or sediment deposition, depending on the quantity of water available, the nature and quantity of sediment in the system, and also on the change in topographic gradient between particular locations. Soils in Britain are also relatively transient structures, with development times of hundreds to thousands of years. Their characteristics are of significance in that they are a major determinant of surface and near-surface hydrology and patterns of interflow (see Section 5.6), as well as being a factor constraining the range of ecosystems likely to develop in the area of interest [177]. The processes leading to soil formation and erosion and data on erosion rates have been reviewed on behalf of Nirex [178].
The lithosphere plates that make up the Earth’s crust are in constant motion. Rifting and sea floor spreading are occurring at extensional active plate margins (e.g. spreading at the Atlantic mid-ocean ridge), whilst collisions and lateral movements between plates occur at other locations. In the long-term future (>10⁶ years), these tectonic processes will modify the position of the land surface and coastlines, relative to a deep geological repository. Erosion and sediment infilling will further modify the topography of regions of the UK due
Box 6.2. Relevant information on current biospheres

Data and information for the present day climate at the two sites in the UK recently of interest for a potential disposal facility (Sellafield and Dounreay), and for a number of relevant current day analogues for the main climate states that will develop with both short- and long-term climate change, have been collated for Nirex by the Climate Research Unit of the University of East Anglia [152, 154]. Selection of appropriate analogue climate stations has to be based on knowledge of a specific site. This is because actual climate data must be appropriate for the latitude and altitude of a specific site and other features which influence the more local nature of the climate within a particular climate state, such as distance from the sea, must also be considered. Since Nirex has already developed the methodology to select and extract analogue information, its application to a future site selection programme could be readily applied. The methodologies developed by Nirex were subject to peer review and discussion at a specially convened workshop in 1989 [116]. Since that time, many papers have been presented at other national and international meetings e.g. [159, 199, 200]. Work is continuing to keep abreast of new developments in interpretation of causes of climate change and in modelling approaches. For example: implications of new data for modelling the effects of anthropogenic greenhouse gases; interpretation of data from new, deep ice cores from Greenland; identification of the short-term dynamics of past climate change and implications of evidence from calcite in Devils Hole, Nevada for climate change time scales and processes. All this work will provide a sound basis for providing climate change input for any site selection programme or biosphere assessment following the site selection process.

Site-specific information has been collated on the soil types and associated land use patterns for the Sellafield area [179]. In combination with generic data on soil types for different climate states, this has enabled the collation of a database of sorption values and other relevant parameter values for different soil types for use in modelling [179, 234]. To understand more fully specific aspects of the biosphere that could influence radionuclide behaviour in the surface environment, Nirex has also commissioned reviews of the literature and assembled data on topics such as:

- the retention and mobility of artificial radionuclides in soils, including generic soil erosion and re-suspension rates [239];
- the organic matter content of soils with different climates and land use practices [239];
- the action of burrowing animals and deep rooted plants on soil turnover [180];
- the generation of soil gases [181];
- the processes operating in marine and estuarine environments [234];
- solute transport in the near-surface environment [211]; and
- soil-plant radionuclide interaction [224].

Nirex has assembled appropriate information relevant to current biosphere transport processes from surveys conducted by the Ministry of Agriculture, Fisheries and Food on local, regional and countrywide food consumption patterns. Such information gives a basis for consideration of the types of food and consumption rates for calculating doses from ingestion of food containing radionuclides by potentially exposed humans in the future [144, 242].
the far-field effects of compression in the Alpine belt, continuing subsidence of the North Sea basin and crustal deformation during and after the last glaciation (e.g. [182]).

6.2.3 Past, present & future biospheres

It is acknowledged that, by the time repository-derived radionuclides in groundwater begin to reach the biosphere, the climate could be quite different to that of the present day. The study of the present day biosphere at a potential site will, nonetheless, form an important part of a programme of biosphere research. There are a number of reasons for this. Present day conditions could persist for longer than 10,000 years and, even if conditions persisted for a lesser time than this, similar biosphere conditions to those found today could exist in a future interglacial. Considerations such as these (and others) make it inevitable that performance assessments will consider radionuclide releases to a biosphere analogous to that of the present day. Other reasons are that the present day biosphere constitutes the starting point for all future biospheres at a site and that characterisation of the present day biosphere will be needed for use in ‘conventional’ (i.e. not post-closure) environmental impact assessment. Consequently, present day, site-specific biosphere data will be required (Box 6.2).

In considering possible future biospheres, the main starting points will be the current biosphere, possible future climate sequences (e.g. Figure 6.4) and possible future landform changes. Consideration of appropriate current day climate analogue stations: sites that have characteristics (e.g. temperature, precipitation, latitude, aspect, elevation) analogous to the ones of interest will suggest possible future biospheres (Box 6.2). In addition, classifications of currently existing climate states and the corresponding ecological systems are widely available e.g. [183, 184].

Figure 6.4 - Past and future climate changes
This information, together with an understanding of the mechanisms of change, provides a framework for describing the possible future evolution of the biosphere at any UK location. There are two main approaches that can be used to represent future environmental systems [185]. The first divides the future into a series of discrete climate states that can be independently assessed, with each discreet state assumed to apply constantly. The second approach attempts to simulate the whole system as it changes with time. Whatever approach is used, the difficulty of representing future biospheres is recognised in many other national [e.g.186], international [187] and European [188] waste disposal research programmes. For this reason, Nirex has been very actively participating in the BIOMASS project, an IAEA co-ordinated research programme. The aim is to develop an internationally accepted methodology for identifying, describing, and representing assessment biospheres (i.e. biospheres used in performance assessments) together with a set of Reference Biospheres – predefined biosphere conditions suitable for use in assessments [185, 189, 190, 191, 192, 193, 194] (Figure 6.5).

It is not expected that Reference Biospheres will replace site-specific biospheres. Rather, the set of Reference Biospheres will complement the site-specific cases by providing an internationally agreed standard against which the site-specific cases may be compared.

Figure 6.5 - Reference biosphere developed as part of the BIOMOVS complementary studies

To facilitate the construction of future climate scenarios, Nirex is also developing a climate modelling capability that is appropriate to long-term (to $10^6$ years) assessments. There are several kinds of climate change models, each type being appropriate for a certain type of investigation. For example, energy balance models (EBMs) are generally used for scoping calculations. Such models are usually one-dimensional (latitude), with no representation of vertical and atmospheric dynamics and with heat transfers being dealt with by a diffusion approximation.

A second category of climate models includes sophisticated and computationally highly intensive climate models called general circulation models (GCMs). These are used for
assessing short-term climate changes, for example, the impact of the increase in atmospheric concentrations of carbon dioxide and the other ‘greenhouse’ gases on climate. Such models are generally only used to simulate climate conditions over a period of a few decades, not the hundreds of thousands of years required for radiological assessment studies. Furthermore, they cannot predict the ice-sheet distribution or its evolution that occurs as climates move from cool to cold conditions.

A third category of climate model is termed Dynamic Statistical. Models of this type are intermediate in complexity between EBMs and GCMs as they incorporate certain physical first principles, but also parameterisations based on observed statistical relationships linked to climate change. For example, it has been observed that CO₂ levels are low in glacial periods and elevated in inter-glacials and a statistical relationship between CO₂ and insolation can be established. The use of Dynamic Statistical models provides computational efficiency and therefore the models are appropriate for investigating long time periods.

Professor Berger (from the Universite Catholique de Louvain-la-Neuve, Belgium) and his co-workers, have been developing a Dynamic Statistical model based on reconstruction of changes in global ice volume observed in the last glacial-interglacial cycle [195, 196, 197, 198]. This Louvain-la-Neuve model is zonally averaged (5 degree latitude) with a northern hemisphere, single ocean basin representation, appropriate for investigating climate change over time scales represented by glacial/inter-glacial cycling. Each new version of the model has incorporated more features that have resulted in improved climate reconstruction (Figure 6.2) capability when compared to proxy data from the different study disciplines. Nirex uses the models of Berger and his colleagues to scope long-term future climate states [199, 200], as illustrated by Figure 6.4.

Other specific modelling tools to be used to represent future biosphere states and being developed by Nirex include those listed below.

- A cold regions near-surface modelling capability using SHETRAN. This is a physically based, spatially distributed finite-difference model for coupled surface/subsurface water flow. It includes multi-fraction sediment transport and multiple, reactive (e.g. radionuclide) solute transport in aquifers and river basins.
- An ice sheet modelling capability using a robust and tested series of numerical approximations to represent the strongly non-linear processes that operate during ice sheet development.
- A methodology and associated software to record a large number of features, events and processes (FEPs) that contribute to the biosphere system e.g. [201].
- A methodology for structuring the FEPs to provide a systematic framework for identifying the FEPs that form part of the natural evolution of the system and alternative potential evolutions in order to construct cases, or scenarios, for assessment [202].

It is not sufficient just to represent the physical, chemical and biological components of future biospheres. In addition, human communities also must be represented in order for radiological risk estimates to be calculated. However, future development of human society represents a significant uncertainty because of the impossibility of trying to predict future human behaviour. The general internationally agreed approach is to adopt the assumption that the range of future behaviour will be similar to that of today. In the UK, the National Radiological Protection Board therefore recommends that potentially exposed groups of people are based on current day lifestyles [203]. This method can be extended to potential
future biosphere communities by considering people living in the different climate states
found today. The most cautious approach also assumes that such communities make the
maximum use of food and other products derived from the area where radionuclides emerge
into the biosphere. Nirex has therefore adopted a three-pronged approach to representation
of human groups that potentially may be exposed in future biospheres:

- utilisation of current day local survey data on habits, lifestyle and food consumption e.g.
  [144];
- collation of information for subsistence type communities in Boreal and Tundra climates
  as analogues for future climate states [172]; and
- contribution to the IAEA BIOMASS international discussions on representation of
  potentially exposed groups in performance assessments [193].

All of this work is applicable to any site or site-selection programme.

It is the intention of the BIOMASS project to provide a protocol for use in the biosphere
data collation, review and selection exercises. The protocol would ensure that there was a
well-documented audit trail concerning the selection of data for biosphere representations.
Research and development performed to date has been very useful input to the protocol.
However, consideration will continue to be given as to how best to deal with issues
concerning spatial and temporal variability and the uncertainty of data. Methodologies to
deal with scaling also need to be refined

The problem of scaling in the biosphere can be exemplified by the use Nirex make of the
Louvain-la-Neuve climate model. Simulations from the model provide results for fairly
large global segments (5 degree latitude) that are based on an artificial geography. Various
approaches to downscaling the results to regional or local scales have to be considered and
two broad alternatives are possible. First, the use of nested models; secondly, use of
empirical relationships. Suggestions for appropriate methods to be adopted have been made
[199]. Climate data is one example of where thought must be given to the downscaling of
information when considering a region or even a local area around a specific site. This issue
will apply to many facets of the biosphere characterisation studies when moving from
generic considerations to site-specific ones.

6.3 Behaviour of radionuclides in the biosphere.

The biosphere acts as a receptor for radionuclides that migrate through the geosphere. The
two main transport modes are in groundwater or as gas. The transfer of radionuclides
between the geosphere and biosphere is of key importance to repository performance as it
will determine the concentrations and form of radionuclides in the immediately accessible
environment. Once in the biosphere, there are many processes that affect radionuclide
behaviour. Information is therefore required in terms of radionuclide concentrations in the
transport medium (e.g. the groundwater) and how these concentrations are delivered to the
receiving medium in the biosphere (i.e. soil, aquatic sediment, or water body).
6.3.1 Transport in Groundwater

Within the Nirex repository concept, and in many others, a key transport mechanism for radionuclides would be within groundwater as it flows through the repository and up through the geosphere into the biosphere [8, 12, 173, 187, 204, 205]. For transport in groundwater, the near-surface hydrological system is a major factor in determining the distribution and transport of radionuclides in the biosphere following emergence from the geosphere.

Much effort has been invested in understanding near-surface water flows and how to representing them in suitable models. The characterisation of Quaternary deposits can provide much background information for this, because the nature of the Quaternary deposits affects both groundwater recharge and discharge. Complete characterisation of all deposits, and the full representation of their behaviour in a model is unrealistic. The objective has therefore been to develop simplified but realistic models for each potential future climate/biosphere state and to provide representative data for the main processes involved [206]. At Sellafield, data were assimilated to provide:

- the required descriptions of near surface hydrogeological properties for biosphere radionuclide transport calculations;
- data to define the boundary conditions between the groundwater flow models and the near surface hydrology models; and
- suitable parameter values for the safety assessment calculations concerned with groundwater flow and radionuclide transport.

Both catchment scale and regional scale near-surface models for Sellafield were developed [173, 207]. Using these models, various near-surface biosphere processes can be examined (Figure 6.6), for example, how changes in climate affect the direction and magnitude of near-surface water flows (e.g. due to permafrost), the amount of water available for infiltration and surface water runoff, and groundwater discharge patterns.

The Nirex catchment scale model is SHETRAN and is based on a model called SHE developed by the Danish Hydraulic Institute, the British Institute of Hydrology and SOGREAH, a French institute [208, 209, 210]. The SHE model has been tested by application to catchment areas in England (Slapton Wood) and mid-Wales (the Wye catchment), and in a variety of countries including New Zealand, Switzerland, Thailand, USA, France, Denmark, Italy, India and Germany. The model has been adapted for Nirex by the Water Resource Systems Research Unit (WRSRU) of the University of Newcastle to include: contaminant transport (hence the name SHETRAN) in both solute and sediment phases. The model includes treatment of radionuclide decay and ingrowth, storage and recycling, variable saturation of the unsaturated zone, and lateral movement of water in the saturated zone: see [172].

Since the model is physically based, the various parameters can be measured directly in the field or in laboratory experiments. In order to test the model, Nirex has collected appropriate data at different sites both in the UK and France (Figure 6.7) and a blind test validation methodology has been developed for both groundwater flow and solute transport. To parameterise and test the model, catchments have been chosen to give data for different types of climate and include a snowmelt catchment (sited in Idaho, USA) for cold climate modelling, a Mediterranean catchment (Rimbaud in France) for modelling a future warm climate, and Temperate catchments (Slapton Wood and Calder Hollow, UK). Two blind validation exercises have been carried out: for flow [172], in the Rimbaud catchment, and for solute transport [211], at Calder Hollow. (A blind validation is one in which the model is
used to predict the outcome of an experiment without sight of the experimental results). SHETRAN has also been applied by many different organisations for many different physically based river catchment modelling problems in Europe. This gives confidence that the methodology and data applications are suitable for future safety assessments.

**Figure 6.6 - Processes simulated within the SHETRAN model**

6.3.2 **Transport as Gas**

Issues associated with the formation [76, 212] and movement [119, 213] of gases through the geosphere have been dealt with in Section 4 and will not be repeated here. The main gases that might be released from the near-field and geosphere into the biosphere are carbon-14, hydrogen, tritium (H-3) and radon [214]. The different chemical forms of these gaseous radionuclides and their potential impacts in the biosphere have been studied, both in the UK [214, 215, 119, 216, 74, 77, 217, 218] and in other national repository programmes (e.g. in Sweden [219] and Switzerland [220, 221]). The radiological impact on humans of exposure to the gases through inhalation, external irradiation or skin absorption (where relevant) can be taken into account in safety assessments since international recommendations and appropriate dosimetric models are available from the International Commission on Radiological Protection.
For carbon-14, a special model has been developed by Nirex to assess the impact from incorporation of the radiocarbon into methane and the potential transfer to humans via food chain pathways. This model, RIMERS, [77] simulates the fate of carbon-14 entering the soil zone as methane and the subsequent pathways. The impacts that would arise from tritium or radon releases and build up in buildings have also been assessed. Nirex has also given consideration to the possibility that gases such as hydrogen and methane can be flammable in air. Studies have been carried out of the potential flammability hazard in buildings from the accumulation of gases generated within the repository [77].

While the models developed to quantify the biosphere impact of repository generated gas are not dependent upon a particular site location, the output of some of the models does depend quite strongly on the degree of localisation of the releases. This information will be site-specific and would need to be obtained from fieldwork at the site.

*Figure 6.7 - Calder Hollow studies*
6.3.3 Radionuclide Interactions in the Biosphere

Once radionuclides have been transported to the biosphere, it is important to know how they will behave in the different components of the system. The particular components of interest are: soils and sediments; plants and animals; and aquatic systems.

For a number of years Nirex has commissioned an extensive programme of experimental research and associated modelling on how radionuclides are transported from a contaminated water table up through the soil (Figure 6.8). This large programme of experimental work has been performed by Imperial College using soil lysimeters and soil cores [222, 223, 224, 225, 226, 227, 228].

Figure 6.8 - Conceptualisation of soil-plant radionuclide transfer processes
Such work is required because previous knowledge of how radionuclides are transported in the biosphere came mainly from experimental sampling following weapons testing and the Chernobyl accident. Whilst all this information was useful, information was required not just on atmospheric deposition and downward migration of radionuclides in soils, but also how they are transported up through soils. Results from these lysimeter studies are extremely useful for developing research models of the processes involved in radionuclide transport in soils and also for input to the biosphere assessment models. The data that have been collated have been so useful and important that they were used as the basis for a model test exercise in an international collaborative project (BIOMOVS II) for the testing and validation of soil process models [229].

Nirex has a number of databases that provide detailed information on the physical and chemical characteristics of all the potential radionuclides that may be present in the repository wastes and how they interact with biological organisms. Of particular importance is a knowledge of the physical half-life, the solubility of different chemical species of a radionuclide, the extent to which a radionuclide can interact with rock surfaces or particles of soil or sediment in order to retard its transport through a particular medium, and the human dose that can result from ingestion, external irradiation or inhalation exposure modes. The majority of such data are well established. Relevant data for the behaviour of the radionuclides in terrestrial and aquatic ecosystems have also been collated. This information has been based on nationally and internationally recognised data sets e.g. [230, 231, 232, 233] and specifically commissioned reviews for soils and aquatic systems, including [234, 235, 236, 237].

In addition, a number of in-depth reviews have been undertaken for Nirex on the behaviour of specific radionuclides known to be important in performance assessment. Reviews have been conducted for: chlorine, technetium, iodine, neptunium, radium, protactinium, tin and carbon [238, 239, 240]. For all of these radionuclides, data have been collated for the chemical form of the radionuclides in water and soils, how the radionuclides interact with soils or sediments and how they are taken up by plants or animals. Information has also been reviewed on how radionuclides may be retained, taken up and translocated in vegetation following deposition of contaminated water onto plants [241].

The UK Environment Agencies [16] identify the need to consider impacts on non-human species [16, paragraph 6.27]. Nirex has already done some work to address this issue [242, 243] and work is ongoing in various countries (e.g. Canada and Sweden) as well as by the IAEA.

6.4 Summary of knowledge base and capabilities.

Methods have been developed for modelling the important processes that contribute to understanding groundwater transfers between the geosphere (within which the site is located) and the biosphere (e.g. the near-surface hydrogeology and hydrology). In addition, the explicit simulation of time-dependent processes (such as ice sheet development and retreat) may need to be considered in the context of specific sites. The continued international research and development of modelling techniques will contribute in this area. Information required to characterise the biosphere has been reasonably well established through experience and international co-operation (Figure 6.9).
The extensive experience gained characterising the complicated Sellafield Quaternary sediments can be readily applied to any future site investigation, as the skills already obtained in analysis and interpretation of samples will be transferable to any other site. Similarly the techniques used to understand Quaternary environments at Sellafield can be applied to other localities.

Investigations of the biogeochemical processes involved in radionuclide transfers between soil and plants are continuing in the Nirex biosphere research programme. Lysimeter and column experiments have been augmented by modelling studies and an increased understanding of radionuclide transport for key elements in a range of soil types has developed.

Nirex has been actively participating in the BIOMASS international programme being conducted under the auspices of the IAEA and will be well placed to apply the generic methodology and protocols in the context of the UK regulatory framework. The approach for characterising the biosphere is dependent upon the approach adopted for the future biosphere representation in the performance assessment. In the IAEA BIOMASS Reference Biosphere methodology it is recommended that the context for the performance assessment is explicitly laid out at the outset [190]. Biosphere representation methods would therefore need to be stated at the beginning of any new site investigation programme and, if possible, this should be agreed with the Environment Agencies beforehand. This would then guide the assessment rationale to be used and guide the type of information and data that should be collected. Following selection of a specific site, the assessment context would be modified as necessary to reflect site-related requirements.
7 POST-CLOSURE PERFORMANCE ASSESSMENT METHODOLOGY

7.1 Current position

Post-closure performance assessments (‘performance assessments’) of deep geological disposal systems have been carried out for over twenty years, progressively growing in sophistication and in their capability to incorporate a wide range of data (Figure 7.1) so as to simulate the detailed behaviour of the multiple barrier system. They are integral to development of a repository programme based on deep disposal. Performance assessments are based on the scientific understanding of the behaviour of a backfilled and closed repository system. They typically use models to provide quantitative evaluations of the behaviour of the repository system. These evaluations can be compared with regulatory standards. Performance assessments are therefore an important component of the science underpinning deep geological disposal and the models on which they are based are important tools for integrating the multidisciplinary scientific research into a cohesive representation of the repository system (Figure 7.2).

Figure 7.1 - Inputs to performance assessments
Many important safety assessments for deep repositories have been published over the last ten years from different countries and in different contexts: to demonstrate the performance of disposal concepts, to illustrate performance assessment methodology, to evaluate the performance of potential repository designs at specific sites or to meet regulatory licensing requirements.
In this period substantial developments have been made in the ability of performance assessments to identify and incorporate appropriate descriptions of the system. In particular, these developments include systematic approaches for scenario development based on the analysis of features, events and processes (FEPs) and the explicit handling of uncertainty. An evaluation of ten performance assessments [100] identified other significant advances in:

- dealing with large site data sets and more formal methods of reduction of data for use in assessment models;
- more sophisticated use of geochemical programs and data to simulate pore water composition and evolution and to arrive at element speciation and solubility equilibria;
- use of three-dimensional models of groundwater flow, including density and transient effects, and use of spatially-variable models of hydrogeological systems, based on site data;
- greater understanding of the transport of contaminants through fractured rock and unsaturated rocks;
- better based models of particular processes, e.g. treatment of colloids, gas-mediated releases;
- more sophisticated use of probabilistic programs including representation of time-dependent processes and events; and
- application of more rigorous quality assurance procedures for assessment decisions, control of input/output data sets, and program development.

The general view resulting from these performance assessments and from experience prior to the 1990s [100] is that performance assessment methods are currently available to evaluate adequately the potential long-term radiological impacts of a carefully designed waste disposal system.

7.2 Systematic treatment of uncertainty.

There will always be uncertainties within performance assessment calculations. In this context, uncertainty means a lack or limitation of relevant knowledge. It is often difficult, for instance, to be certain about how the geological environment arrived at its current state, given the multitude of alternative explanations that can usually be offered. This is important because the evolution of the site to its current state is often used as an indicator of possible future changes.

Sources of uncertainty in assessing the performance of a potential repository include:

- uncertainty over the future evolution of the repository and the environment;
- uncertainty about future human behaviour which may be of consequence in terms of potential radiological doses;
- uncertainty in the accuracy of the models used to represent the repository system; and
- uncertainty in the data and parameters required for the models, including scarcity or lack of data.

The first two types of uncertainty can be addressed by evaluating a range of likely future responses of the disposal system to different scenarios (events, and evolution of the system and its environment) and the consequences of this behaviour in terms of possible radiation
doses or risks to people. In order to calculate potential radiological risk for each scenario it is necessary to consider the relevant features, events and processes (known as FEPs) which could affect the performance of a repository, either now or in the future. Comprehensive FEP analysis programmes have been undertaken by many national programmes and are the subject of intensive activity in international collaborative programmes.

Different scenarios will be appropriate for different repository designs and for different sites. The rocks surrounding the repository and the surface environment will affect the nature of groundwater flow, the passage of gas and the likelihood of direct human intrusion or of wells being sunk near the repository. These are the main routes that could lead to potential exposure to radioactivity and that form the basis of a performance assessment. The nature and relative magnitude of the associated risks will therefore vary, depending on the site where the repository is located.

Uncertainty in the models can be addressed by considering alternative models and by using the models to make predictions that can then be tested against observations (i.e. validation). This points to the potential importance of “soft data” and information not necessarily included in the models to overall confidence in the results of the performance assessment.

The approach adopted for dealing with uncertainty in data is to establish the range of possible values for each uncertain parameter. Typically this range is based on measured values, supplemented by the judgement of suitably qualified experts, and takes into account any scarcity of data or bias from measurements. The uncertainty is described by a ‘probability density function’, which describes the probability that the parameter will have a particular value within the assigned range of possible values (Figure 7.3).

*Figure 7.3 - Probability density function*

When running the computer models it is possible to sample values from the probability density functions for each of the uncertain parameters. The models can be run many times, sampling a different set of values each time. This is known as a ‘probabilistic safety assessment’, or PSA, approach [244].

In performance assessment modelling it is often necessary to make a number of simplifying assumptions, either because insufficient data are available or the modelling capability
cannot represent some feature of the repository system in full detail. The aim is to address issues as realistically as possible, whilst erring on the side of caution. Therefore, many simplifications involve taking a conservative view whereby an assumption is made such that radiological dose will be over- rather than under-estimated.

7.3 Simulating time-dependent processes over long timescales

Performance assessments carried out by Nirex to date made use of a suite of computer models of groundwater flow and radionuclide transport [8], which were used to calculate radiological risks to potentially exposed individuals as a function of time. However, the models were not able explicitly to incorporate variations over time of model parameters, such as material properties or flow boundary conditions. So, for example, it would be possible to examine the effect of different repository pH values, but not to allow pH to change over time. Similarly, the effect of the presence of an ice sheet could be examined but not the effect of its growth and retreat. Of the two types of time-dependent change, material property changes and flow boundary changes, it is probably the latter that has the greater potential to be significant. The level of significance could be strongly site specific.

To address this potential shortcoming a programme of work was launched by Nirex in 1994 to develop a time-dependent software framework. This software framework was intended for utilisation in future work undertaken as part of the iterative assessment approach. It was originally anticipated that the new software would be available for use in the preparation of a detailed performance assessment that would be submitted to the regulatory authorities in support of a planning application for a deep waste repository at Sellafield, if the results of the RCF programme had given sufficient confidence in the suitability of the site.

Given the importance attached to time-dependence by members of the scientific community, work on the development of time dependent modelling capabilities has continued beyond the RCF decision.

7.4 Current approach to performance assessment and model development

Experience in developing performance assessments for a potential repository at Sellafield and the generic issues identified above have contributed to the development of a modified framework for performance assessment. The experience of developing the Nirex 95 and Nirex 97 assessments has been incorporated into this framework, as well as a systematic FEP analysis approach to the development of conceptual and numerical models using underpinning scientific knowledge. The resulting approach has the potential to enable many of the issues identified above to be addressed in any future repository evaluations. In addition, the approach is designed to improve the traceability of performance assessment modelling.

The performance assessment approach is to identify all FEPs that are significant for the long-term performance of a repository, and from an analysis of these FEPs to identify a range of scenarios (events, and evolution of the system and its environment) which could have an impact on safety [201]. Many of these scenarios may have a low probability of actually occurring in the future. Because of the uncertainty regarding future events, it will be necessary to consider a range of alternative evolutions, or scenarios, for the repository system. In the Nirex approach, it is proposed that the performance of the repository can be assessed by considering a ‘base scenario’ that represents the anticipated ‘natural’ evolution of the repository (those FEPs which are almost certain to occur, such as climate change and fundamental physical and chemical processes) and a range of variant scenarios.
(incorporating those FEPs which are less likely or unlikely to occur, such as large earthquakes and certain human actions).

*Figure 7.4 - The Nirex five stage approach to model development*
A suite of documents has been developed that describes the Nirex model development programme that underpins this approach to performance assessment [201, 202, 245, 246] (Figure 7.4). The programme has been designed to provide a clear audit trail from the identification of significant FEPs, to the models and modelling processes employed within a detailed performance assessment. A five stage approach has been adopted, which provides a systematic framework for addressing uncertainty and for the documentation of all modelling decisions and assumptions.

Stage 1: Analysis – the compilation and structuring of a FEP database;

Stage 2: Scenario and Conceptual Model Development;

Stage 3: Mathematical Model Development;

Stage 4: Software Development;

Stage 5: Confidence Building.

The foundation of the process is the identification and analysis of those FEPs relevant to the long-term safety of deep geological disposal of radioactive waste. A key component of the analysis of these FEPs is the development of the Master Directed Diagram (MDD), which is a structured diagram showing elicited FEPs and the key relationships between them (Figure 7.5). Underlying the MDD is a FEP database, providing a description of each FEP. The MDD is used to identify a base scenario (a broad and reasonable representation of the natural evolution of the system). Modelling requirements for the representation of the base scenario are identified, and a methodology for identifying and characterising alternative, ‘variant’ scenarios, is developed and applied [246]. Modelling requirements for the variant scenarios would be identified using a similar process as applied for the base scenario.

Figure 7.5 - Schematic illustration of selected FEPs on the structured FEP diagram
The groundwater and gas pathways form part of the “base” scenario, whereas human intrusion and natural disruptive events are treated as variant scenarios since they represent events that may or may not occur at some point in the future. The structured approach to FEP analysis, explains how these scenarios may be defined so that they meet the regulatory requirement of encompassing all situations which could be relevant to the performance of a repository. The overall approach is generically applicable to any long-term performance assessment. However, the implementation of the approach, in particular the FEP analysis and conceptual model development stages require specific information on particular sites and repository design. The approach is also consistent with current thinking about how to build confidence in a performance assessment, summarised recently by the NEA.

The use of this approach therefore defines the scientific information required to robustly support a performance assessment considering alternative scenarios.

To date, the scope of the FEP analysis work has been focused on the demonstration of a methodology, rather than a complete implementation of the approach. As a practical demonstration of the FEP analysis methodology, a base scenario and a number of variant scenarios have been identified from analysis of the MDD and underlying FEP database. Conceptual models have been developed for the base scenario. In preparation for a detailed performance assessment it would be necessary to develop any additional conceptual models required to represent the variant scenarios and to ensure that all conceptual models are appropriately represented in assessment software.

The major benefits of this proposed approach are:

- the ability to demonstrate a comprehensive approach to the consideration of all issues of potential significance to the long-term post-closure performance of a repository;
- provision of an audit trail for all decisions taken during the safety assessment modelling process; and
- demonstration of a clear basis for the overall presentation of a detailed safety assessment.

The methodology described above has been subjected to peer review by an international review team drawn from waste management organisations and regulatory bodies under the auspices of the Nuclear Energy Agency. The review group concluded that, although elements of the approach are still being developed, the methodology was potentially sound and, with some development, could find acceptance by the wider community of radioactive waste management organisations and stakeholders. The review group recommended that Nirex more comprehensively and transparently document the methodology.
8 CONCLUSIONS.

In Chapters 4, 5, 6 and 7 the knowledge base underpinning deep geological disposal was presented. Key scientific questions requiring consideration as part of a repository development programme were identified. In this Chapter, conclusions are drawn about Nirex’s view of

(i) the current status of the science underpinning deep geological disposal,
(ii) issues or partial issues that remain outstanding and
(iii) the ability to proceed with a repository development programme should that be considered desirable.

8.1 Current status of the science.

The key questions relevant to the engineered barrier system, the geosphere and the biosphere have been presented in Chapters 4, 5 and 6. In addition, Chapter 7 summarises the development of performance assessment methods that can be used to integrate the underpinning scientific information into an evaluation of long-term repository safety. In very general terms, there is a wide range of viable options for the deep geological disposal of long-lived wastes, and most of these options are supported by an established conceptual basis and tried and tested tools and techniques for developing repository proposals and evaluating their performance.

Nirex believes that a basic understanding of the science of deep geological disposal has been established. Of course, as with any area of science, it is expected that detailed understanding and methodologies will continue to improve. The current status of the science is summarised below.

8.1.1 Engineered Barrier System

Much work has been carried out on waste immobilisation and migration within the engineered barrier system, and its evolution over the timescale of the repository. In the UK, this work has primarily focussed on a cementitious repository for ILW/LLW. However, information on the use of an alternative backfill (bentonite, crushed salt) could be obtained from other research programmes (e.g. in Switzerland, Sweden and Germany) to support a UK research programme into alternative repository designs for UK wastes.

Many elements of the existing research on the design of engineered barriers are generally transferable to the development of specific repository proposals for low and intermediate level wastes within the UK. The existing information would, of course, need to be supplemented if the range of wastes to be disposed of were extended (to include, say, high-level waste). Additionally, other elements of the research into the engineered barriers are specific to a particular geological environment. Although the underlying concepts will be generally applicable to other similar environments, site-specific data would be required to evaluate and quantify the extent of interactions between the engineered barriers and the surrounding geosphere.

8.1.2 Geosphere

The evaluation of the geosphere for any specific repository development proposals must be site specific. There is an extensive array of site characterisation field techniques available for a wide range of different rock types. Experience from the extractive industries has been modified for specific application to sites under consideration for radioactive waste disposal.
and in many cases novel investigation techniques have been developed and applied. The approach to deploying site characterisation techniques will vary from site to site.

There is considerable depth of international experience in methods to analyse and use information from site investigations in evaluating the viability of specific repository development proposals. In the UK, these methods have been extensively applied to the evaluation of a fractured basement situated under a sequence of various sedimentary rocks. Information from a different site will be different. However the processes by which the, often complex, geological information is reduced to manageable proportions and used to develop conceptual and numerical models of the geosphere are transferable to any site.

The low levels of groundwater flow that generally prevail at a potential repository site mean that it can be difficult to obtain representative samples of groundwater for chemical analyses. Some chemical measurements (in particular pH and Eh) are more vulnerable than others to contamination during the sampling process. Some work is required to develop and apply sampling techniques in order to obtain the necessary suite of chemical data at an appropriate stage in a repository development programme. In addition, initiatives are being put in place internationally to develop methods for interpreting a range of chemical and mineralogical information to determine past groundwater history (paleohydrogeology) and to apply this knowledge to build confidence in conceptual models of groundwater flow.

Representative samples are generally easier to obtain from underground facilities. A number of other issues regarding the geosphere are more amenable to underground investigation than by drilling from surface. It is therefore generally assumed that a phase of underground research will be undertaken as part of a repository development programme. This provides an opportunity to test conceptual models developed as a result of investigations from the surface. There are a number of examples internationally of such underground research facilities. In the UK, methods of excavating and experimenting in such a facility, and more importantly of integrating the data from that facility into a programme of model development were established for the (now terminated) repository investigation programme at Sellafield. These methods would be transferable to another site, although the detailed programme of experimentation would need to be tailored to site-specific conditions and conceptual models.

Underground construction will disturb a site and it is important to establish that the baseline conditions are understood prior to such disturbance. Experience at Sellafield showed that baseline conditions could be defined and, through the use of peer review, widely accepted. This approach could be applied at another site.

8.1.3 Biosphere

Because of the need for conservatism in the treatment of the biosphere, and the dependency of radiological risk on assumptions regarding the future, the issues relevant to characterising and evaluating the biosphere within a repository development programme are dependent on the way the biosphere is treated within repository performance evaluation. It is therefore important to establish and agree the proposed treatment of the biosphere early in a repository development process.

Current generic international research into the use of biosphere models in performance assessments is being focussed through the IAEA BIOMASS project. This generic research base would need to be adapted to any specific repository development programme. This will involve, in particular, the collection of site-specific information to support environmental impact assessments and to understand past temporal variations in climate and landform. Methods and techniques to achieve this are well established and have been
applied rigorously within the UK during the investigation of the Sellafield site. Future climate sequences can be constructed using global scale models such as that developed by a team at Louvain-la Neuve. However, for a specific site, global climate needs to be downscaled to account for a more localised geography. Various approaches have been put forward for this downscaling but the work is still in its early stages.

Many of the processes that affect radionuclide concentrations in the biosphere are dependent on assumptions about human behaviour and/or future climate states. These assumptions will generally be common to any site within the United Kingdom and much effort has gone into establishing that the assumptions made are conservative (i.e. will tend to overestimate risk). However, in addition to adopting this conservative approach, the research underpinning the biosphere may also need to evaluate the radiological impact on non-human species. This is an emerging area that may require the collection of new data and the development of new methodologies.

The simulation of radionuclide transfer from groundwater in the geosphere to surface water bodies in the biosphere has received much attention and various methods are available to achieve this. The SHETRAN program adopted by Nirex has been through a validation process and provides a powerful tool for simulating this important transfer process. Internationally, work is ongoing to evaluate the radionuclide transfer processes that result in radiological risks to human and non-human species. The conceptual model established by this work is generically applicable. In addition, the magnitude of radiological risk will be dependent on generic assumptions about future habitats and climates.

### 8.1.4 Performance Evaluations

Performance assessment methods have advanced significantly over the past ten years, and a recent review by the NEA [100] has concluded that PA methods are currently available to evaluate adequately the potential long-term radiological impacts of a carefully designed waste disposal system. In particular, this period has seen advances in the development of systematic approaches for scenario development based on the analysis of features, events and processes (FEPs). It is expected that these approaches will assist assessments to be demonstrably comprehensive, auditable and clear. Clarity is also aided by the use of formal methods for reducing the size of very large data sets so that they can be used in assessment models.

In addition to the development of the FEP approach, recent years have seen advances in the explicit handling of uncertainty in respect to (i) the future evolution of the repository and its environment, (ii) relevant human actions and (iii) data used in the models.

While some aspects of time dependence can be addressed, performance assessment methods are not, in general, capable of explicitly incorporating variations over time of model parameters such as material properties or flow boundary conditions. Of the two, it is the latter omission that has the potential to be the more significant, although the absolute level of significance is likely to be site specific.

### 8.2 Outstanding Issues

Based on the information presented in the preceding chapters and summarised above, Nirex believes that a number of technical and scientific issues – ‘outstanding issues’ - can be identified whose resolution would significantly raise the level of scientific confidence associated with the deep disposal of radioactive wastes.

These issues can be broadly grouped into two categories:
• site-specific data requirements, that can only be fully addressed if a particular site is identified for investigation; and
• more general (i.e. non-site-specific) issues such as those relating to the performance of the engineered barriers.

8.2.1 Site-specific data

There are a number of issues that could only be addressed if a specific repository development programme were initiated. These are issues for which site-specific information is required, for example, the extent of interactions at the engineered barriers/geosphere interface and the geosphere/biosphere interface and the characterisation of the geosphere. Among the issues that would need to be addressed by a site characterisation programme, a few have been identified as outstanding.

• Uncertainties remain with respect to the interactions, over an extended period of time, between the excavations, the engineered barriers and the host rocks. Particular issues are the long-term changes in the mechanical disturbance created by the excavations, the evolution of the chemically-disturbed zone and their coupling to groundwater flow.

• There is, at present, only a limited ability to obtain representative in situ groundwater samples for reactive constituents from very low permeability rocks from surface based investigations. This means that it can be difficult to precisely determine the redox potential of the repository host environment.

• The impact of gas migration is uncertain, particularly in relation to its effect on groundwater movement and the localised release of radioactive gas at the surface. Because gas migration testing has the potential to disrupt the existing groundwater flow patterns, such testing would only be carried out in the later stages of the site investigations.

This review concludes that it would be possible to obtain the requisite information over the course of a carefully structured and managed site investigation programme.

8.2.2 General issues

In addition to the site-specific issues summarised above, there are a number of other issues that may be classed as outstanding.

• Palaeohydrogeological information is seen as central to building confidence in the assumptions made within performance assessments. At the same time paleohydrogeology is an emerging science whose nature is such that it is usually necessary to employ a wide range of arguments before a unique solution can be arrived at.

• While the performance assessment methodology is capable of addressing some key aspects of time-dependent processes (e.g. the effect of different flow boundary conditions), more explicit treatments (e.g. ones that address the change from one flow boundary condition to another) are not yet available. Whether the issue of transitions in flow boundary conditions is a significant one is likely to be a site-specific matter.

• There is uncertainty associated with the evolution over long time scales of the engineered barriers, in particular cementitious materials such as the NRVB and repository seals. It is expected that the use of a wide range of laboratory investigations together with natural and anthropogenic analogues will improve understanding of the relevant long-term processes and so increase confidence in the models.
• Some uncertainty remains with respect to the extrapolation from laboratory conditions to in situ conditions. An example is the use of laboratory sorption and rock matrix diffusion data in performance assessments. This is likely to be resolved through the development of a more thorough understanding of the relevant mechanisms together with appropriate experimentation (including in situ experiments) and the use of natural analogues.

• The degradation of organic materials has the potential to form compounds that, through complexation, may mobilise radionuclides, such as plutonium, that would otherwise have very low mobility. While this issue is now relatively well understood, some important uncertainties remain: in particular, the rate of the degradation, the identification of all the organic complexants that are involved in a significant way and, to a lesser extent, the range of radionuclides that could be affected.

As shown by this report, work to address these outstanding issues is ongoing within the UK national programme in the context of continued evaluation of the generic phased disposal concept.

8.2.3 General principles

More widely, a number of general principles can be identified to improve the scientific confidence in the research undertaken by any organisation involved in evaluating deep geological disposal. These include:

• ensuring demonstrably high quality scientific work at all times;

• the use of multiple lines of evidence, including the widespread use of natural and anthropogenic analogues (environmental features that have arisen as a result of phenomena similar to those being represented in models of the repository);

• adding value by integrating knowledge gained through traditionally segregated disciplines within science and engineering;

• the application of rigorous peer review;

• adopting a clear process of model validation; and

• peer preview, which recognises that a better dialogue is required with the scientific community (and, ideally, a wider range of stakeholders) before starting a piece of scientific research.

These principles provide guidelines to govern the development of scientific research in the future. A key challenge is to apply them and other techniques in a manner that will inspire confidence, not just in particular scientific conclusions, but in the research organisation itself.

8.3 Ability to Proceed

Nirex believes that, although some outstanding issues remain, there is generally work in place nationally and internationally to address them. None of these issues is seen as an overriding obstacle to deep disposal in principle.

A phased programme of repository development would provide many opportunities for a review of the science and associated uncertainties and consultation with a wide range of
stakeholders. Indeed, obtaining an agreed outcome from such iterative reviews of the science could be a determinant of the rate at which the programme proceeds from phase to phase.
9 REFERENCES:


147 GRIP (Greenland Ice-Core Project), *Climate Instability During the Last Interglacial Period Recorded in the GRIP Ice Core*. Nature 364: 203-207, 1993.


192 IAEA, Biosphere System Identification and Justification. BIOMASS Theme 1, Draft Working Document No.6 (IAEA Working Material), 1999.


194 IAEA, Biosphere System Description and Radionuclide Transport Modelling. BIOMASS Theme 1, Draft Working Document No.7 (IAEA Working Material), 2000.


Feedback

Readers are invited to provide feedback to Nirex on this report. Feedback should be addressed to:

Helpline Administrator
United Kingdom Nirex Limited
Curie Avenue
Harwell
Didcot
Oxfordshire
OX11 0RH
U.K.

Or by E-mail to: info@nirex.co.uk