PADAMOT

Palaeohydrogeological Data Analysis and Model Testing

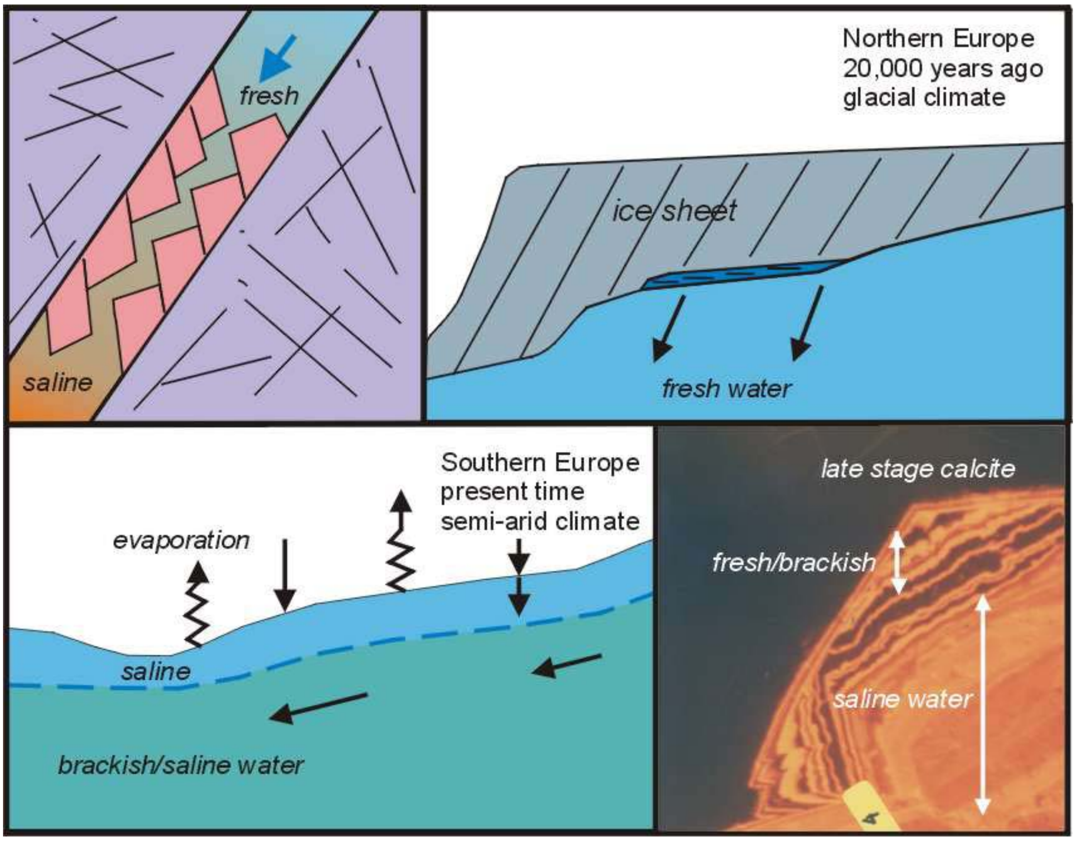
Fifth Framework Programme

# Dissemination and Use of Palaeohydrogeological Results for Safety Assessment

PADAMOT Project – EU FP5 Contract No FIKW-CT2001-20129

Technical Report WP5

January 2005



PADAMOT PROJECT

TECHNICAL REPORT WP5

# Dissemination and Use of Palaeohydrogeological Results for Safety Assessment

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BATH, A. AND DEGNAN, P.. 2005. Dissemination and Use of Palaeohydrogeological Results for Safety Assessment. *PADAMOT Project Technical Report* WP5. 82pp.



Harwell UK Nirex Limited 2005

# Foreword

PADAMOT, ‘Palaeohydrogeological Data Analysis and Model Testing’, is a project within the European Union’s 5th Framework RTD programme in nuclear fission safety (Contract Number FIKW-CT-2001-00129). It aims to improve the understanding of past groundwater conditions that supports assessments of future long-term safety of repositories for radioactive wastes. The project began in December 2001 with a duration of 36 months. The consortium of organisations involved in the PADAMOT project comprises:

United Kingdom Nirex Limited (UK)

Svensk Kärnbränslehantering AB (Sweden)

Terralogica AB (Sweden)

Empresa Nacional de Residuos Radioactivos S.A. (Spain)

Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (Spain)

Intellisci Ltd (UK)

British Geological Survey (UK)

Charles University (Czech Republic)

University of Edinburgh (UK)

Universidad Politecnica de Madrid - School of Mines (Spain)

Safety assessments of proposed repositories for the long-term storage or disposal of radioactive wastes must take into account scenarios for environmental change over the long period of time during which the waste will be a hazard, typically up to one million years into the future. The scientific consensus in a number of countries is that disposing of long-lived and/or higher activity radioactive wastes and spent nuclear fuel deep underground in a 'geological repository' is the preferred option for long-term radioactive waste management. The reasons for preferring this option are that the host rock for a deep repository should provide stable conditions for performance of the engineered barrier system and that the rock mass separating a repository from the surface environment is a further barrier to radionuclide migration.

During the last two million years (the Quaternary Period), global climate has fluctuated between extremes of ice ages and warmer conditions than at present. Over various intervals in the past, large areas of northern Europe were covered by ice sheets and experienced extensive permafrost, whilst southern Europe was sometimes more pluvial (wetter). Consequently, the present-day climate is not representative of the climate that has existed for much of the Quaternary. This natural pattern of climatic fluctuation is expected to continue into the future, albeit modified by the impacts of anthropogenic greenhouse gas emissions. Variations in climate and in other environmental factors may affect future movements and compositions of groundwaters in the vicinity of a repository and thus affect the mobility of radionuclides and the rate of their migration back to the surface. It could be argued, therefore, that present-day groundwater conditions may not be an adequate basis for assessing long-term repository safety. However, if it can be demonstrated that, despite significant environmental change at the surface, groundwater flows and compositions at depth remain stable or change in a way that does not impact significantly on safety, then confidence in repository concepts for disposal will be increased.

PADAMOT has sought to address the following questions. How can such groundwater stability be assessed, with respect to climate-driven environmental change? In particular, what evidence is there that a deep geological repository will eliminate or reduce the effects of extreme changes in environmental conditions in the long term? In seeking to answer these questions, PADAMOT has investigated geosphere systems at various European sites, using analytical methods and numerical modelling.

PADAMOT comprises five work packages (WPs) with the following tasks:

WP1. Convening a preliminary workshop of PA specialists, PADAMOT researchers and other geoscientists on the use of palaeohydrogeology in PA.

WP2. Making palaeohydrogeological data measurements on mineral samples and groundwaters from sites in Spain, Czech Republic, Sweden and UK, using high resolution and high precision analytical methods, e.g. ion probe and laser ablation.

WP3. Constructing a relational database and a public domain website to store data from EQUIP and PADAMOT, accessible to project partners and to external researchers via the internet.

WP4. Developing numerical models to test palaeohydrogeological information interpreted from proxy geochemical, mineralogical and isotopic data, based on understanding of the processes that link the proxy data with climate-driven groundwater phenomena.

WP5. Synthesising project outcomes and disseminating an improved approach to the use of palaeohydrogeological information in the description of FEPs and hydrogeological scenarios for PA.

There are final reports from each of the five WPs plus a Summary report:

Technical Report WP1. The Long-Term Stability of Groundwater Conditions at Repository Sites: Proceedings of the PADAMOT Workshop, Brussels 2002.

Technical Report WP2. Application of Mineralogical, Petrological and Geochemical Tools for Evaluating the Palaeohydrogeological Evolution of the PADAMOT Study Sites.

Technical Report WP3. Design and Compilation of Database: Final Report.

Technical Report WP4. Interpretative Modelling of Palaeohydrogeological Data: Final Report.

Technical Report WP5. Dissemination and Use of Palaeohydrogeological Results for Safety Assessment.

Summary Report. PADAMOT: Palaeohydrogeological Data Analysis and Model Testing – Overview.

*Conditions of Publication*



*Further Information*

Further information on the PADAMOT programme can be obtained from the project website www.bgs.ac.uk/padamot

# Abstract

Work Package (WP) 5 of the PADAMOT project aims at introducing the use of palaeohydrogeological information for the identification of scenarios that are to be considered in Performance Assessments (PAs) of future radioactive waste repositories.

With this objective, WP5 reviews existing safety cases to find out the extent to which palaeohydrogeological information has been considered in carrying out PAs and to see what sort of evidence was available from geochemical studies and how it was used. The review shows that palaeohydrogeology has been used very variably in PA for which a number of possible reasons are discussed. One of those is that palaeohydrogeological information from geochemistry and mineralogy tends to contain many uncertainties and is rarely translated into qualitative parameters that can be used directly in PA. To improve this translation, it is proposed here that interpretation of palaeohydrogeology should focus on input to the consideration (or 'screening') of Features, Events and Processes (FEPs) in the PA process. FEPs provide a context for palaeohydrogeological information that is recognised in PA. However the challenge is to quantify the information which requires interpretative models to be developed (of which there are some examples in WP4). To illustrate the logic, albeit complex, of transforming geochemical and mineralogical measurements (exemplified by analyses carried out in WP2) into information that is usable by PA, a flow chart of data, supporting information, interpretation and calculations is produced.

The interpretation methods that are used to get from geochemical and mineralogical data to palaeohydrogeological information that is useful for screening FEPs are described at a reasonable level of detail. This should assist PA groups in understanding the assumptions and uncertainties that are involved in using information obtained fro applications of geochemistry and mineralogy in site characterisation, as exemplified in WP2.

Geochemistry and mineralogy were used in WP2 to investigate past groundwater conditions at study sites in Spain, Sweden, UK and Czech Republic. The specific aims, strategies and output data in each case are summarised and the significance of the results in terms of support for FEPs is assessed objectively.

Coupled flow-reaction modelling of the Spanish site, Los Ratones, shows that groundwater compositions and secondary mineralisation are potentially sensitive to changes of groundwater recharge rate during fluctuations of climate from warm-arid to cold-humid. The hydrogeochemistry of the part of the groundwater system that is accessible for study is dominated by weathering and dissolution reactions and precipitation predominantly only of clays. Overall, the investigations here have shown geochemical and mineralogical data that reflect present-day groundwater conditions. There are no data that can be clearly associated with the past climate and hydrological variability for which there is a comprehensive archive of microfossil and organic geochemical data in the Cúllar-Baza and Padul sedimentary sequences.

Mineralogical studies at the Äspö/Laxemar area in Sweden have aimed to follow up previous studies at Äspö by investigating the evidence for past meteoric and saline groundwater distributions at Laxemar where the present-day penetration of meteoric water is deeper than at Äspö. Although there are only small amounts of late stage calcite, information from its morphology and distribution indicate both fluctuating salinity at shallow depths and deep penetration of freshwater in the past. This information, though having substantial uncertainties in the chronology and continuing of the calcites, is clearly of qualitative value for FEPs concerning likely salinity changes due to climate and land uplift.

Additional petrographic analyses of late stage calcite in drillcore samples from past site investigations at Sellafield in northwest England have consolidated the findings from previous

work carried out in the EQUIP project. Morphology variations in overgrowths of late stage calcite have suggested that the position of the fresh/brackish-to-saline water transition zone has fluctuated both above and below its present location, but with additional observations the balance of evidence supports the predominance of a slight downward movement, by at most a few tens of metres, of the transition zone over time, i.e. a dominant trend over time of decreasing salinity at any point in this interval. This indicates that a hydrodynamic and hydrochemical response at 300-400 m depth to changes in the surface environment should be considered in FEPs, but also that the distributions of flow directions in the groundwater system has remained fairly stable over the time period represented by the late stage calcites. Data from various instrumental methods for analysing chemical and isotopic compositions of discrete calcite growth zones suggest that the compositions of groundwaters from which they precipitated changed over time. The patterns of variations support the concept that changes in deep saline groundwaters are more attenuated than in fresher up-gradient groundwaters. In these freshwater calcites, contents of the redox-sensitive trace elements Fe, Mn and Ce are correlated which indicates that the fluctuations in compositions are related to changes in palaeoredox conditions. Thus palaeohydrogeological information suggests that FEPs for PA should consider long-term changes of redox, although it is also evident that the scale of change is attenuated in deeper saline groundwaters. The quantitative significance of the observed Fe and Mn variations has been studied in WP4 by geochemical modelling, which shows that absolute and relative changes in Fe and Mn concentrations have non-unique interpretations in terms of redox (Eh) values.

Samples of secondary calcite from the other UK study sites at Dounreay and Cloud Hill pose an analytical and interpretative problem because the amounts of late stage calcite are low. In both cases the calcite morphologies tend to be dominated by that of older secondary calcite on which late stage calcite has precipitated as a veneer. Uncertainty in calcite characterisation means that the significance of the substantial discordance in the depth locations of the transitions of morphology of late stage calcite and of salinity in the present-day groundwater profile at Dounreay is interpreted with much less confidence than for samples from Sellafield. Variations of redox-sensitive trace elements (Fe, Mn, Ce) are less systematic than at Sellafield although there is a general contrast between trace element contents of shallow and deep calcites with more variation at depth. However there is too much uncertainty and lack of reproducibility in these sparse localised data to interpret reliable palaeohydrogeological information. The few stable isotope data from Dounreay calcites tend to repeat the inference from isotope analyses at Sellafield that glacial or cold-climate water volumetrically replaced pre-existing water down to about 450-500 m depth since late stage calcites below this do not have such light $\delta^{18}O$ values.

In summary, Work Package 5 has found that there is a need to incorporate more palaeohydrogeological information into PA in order to improve the credibility of assumptions about stability of deep groundwaters and of estimates of the likely magnitudes of impacts of external changes in scenarios. The most appropriate way to do that is to use palaeohydrogeology to screen and quantify FEPs that are the basis for developing scenarios to be used in PA. Logical approaches to doing this have been illustrated, showing the considerable steps of data acquisition, interpretation and expert judgement that are involved in attempting to quantify information for transfer into FEPs and scenarios. This process of interpretation and expert judgement is usually carried out by means of a narrative assessment of the evidence. A more rigourous approach with ESL has been exemplified here but it is likely that the conventional narrative approach will continue to be used until much more comprehensive palaeohydrogeological evidence than that from geochemistry alone is available.

Narrative interpretations have been abstracted from the geochemical and mineralogical investigations carried out on samples from the various study sites in WP2 of PADAMOT. The principal methods that have been deployed here, i.e. analyses of mineralogical, geochemical, isotopic and fluid inclusion characteristics of late stage secondary calcite, have been found to have a somewhat limited applicability that clearly depends primarily on the occurrence of late stage calcite in adequate abundance for the characterisation to be analytically feasible and reasonably reliable.

Where these conditions obtain, as in the rocks at Sellafield and to a lesser degree at Äspö/Laxemar and Dounreay, a remarkable amount and diversity of data is obtainable. In other rock formations and for other groundwater conditions, e.g. in shallow groundwater environments, and at earlier stages of site investigations before comprehensive drillcore samples are available from deep boreholes, different sampling and analytical strategies are appropriate. Developments of appropriate strategies have been illustrated with the studies at Los Ratones and Melechov.

Modelling - geochemical, hydrodynamic and coupled reaction-transport - is a valuable and sometimes essential tool for quantitative interpretation and for quantifying the associated uncertainties, as illustrated in WP4.

The full significance of the geochemical and mineralogical indicators of palaeohydrogeology, i.e. of past physical and chemical groundwater conditions has not yet been fully realised even in the most advantageous studies. These studies have shown that uncertainties, assumptions involved in 'expert judgement', and calibrations of process models, remain as substantial sources of uncertainties. Nevertheless for some sites, calcite morphologies, redox-sensitive trace elements and stable isotope ratios can provide qualitative evidence of greater or lesser degrees of stability in past groundwater conditions. This evidence should be taken into account in considering whether deep groundwater conditions will be more or less stable in scenarios of future climate changes in safety cases.

# Acknowledgements

Contributions to the review of palaeohydrogeology in PA were made at the preliminary stage of the project by: Andrew Bowden, David Hodgkinson, Peter Robinson and David Savage (Quintessa Ltd); Trevor Hicks, David Bennett, Mark Crawford and Roger Wilmot (Galson Sciences Ltd); Tim McEwen (SAM Ltd); John Black (InSitu Solutions Ltd).

The trial application of the ESL (Evidence Support Logic) method of data evaluation was carried out by Quintessa Ltd. Meetings of the expert panel were facilitated by Mike Egan of Quintessa using the TESLA software tool. Andrew Bowden assisted with the reporting of the ESL exercise.

Pedro Hernán (Enresa, Spain), Ignasi Puigdomenech (SKB, Sweden) and John Smellie (Conterra Ltd, Sweden) are thanked for reviewing the report on behalf of the task partners as a result of which substantial improvements were made. Richard Metcalfe (Quintessa K.K., Japan) carried out an independent review as a result of which further improvements were made.

The support and involvement of Henning von Maravic and Michel Raynal of EC-DG Research is gratefully acknowledged. The work described in this report was carried out as Work Package 5 of the PADAMOT project in the European Union's 5th Framework Programme of RTD in Nuclear Fission Safety, Contract No. FIKW-CT-2001-00129. It was also supported by funds from UK Nirex Limited, ENRESA and SKB.

# Contents

# 1 Introduction

## 1.1 BACKGROUND AND OBJECTIVES FOR WP5

The primary objective of PADAMOT has been to investigate the evidence for or against changes in deep hydrogeological conditions over relevant timescales and to recommend an effective way to use that evidence in safety assessments. The most likely cause of changing hydrogeological conditions over the timescale of safety assessment is the impact of climate change at the boundaries of the groundwater system. Propagation of climate impacts is likely to be attenuated with increasing depth in a low permeability groundwater system; therefore there is particular interest in showing this to be the case and using this information as concepts and constraints in the development of scenarios for safety assessments of deep geological disposal. The main activities in PADAMOT have been (i) the analysis and interpretation of 'proxies' that indicate various aspects of groundwater conditions in the past, and (ii) the development of models that use data from the proxy indicators to produce palaeohydrogeological and geochemical information about past changes and stability that constrains scenarios for future evolution of geospheres at the study sites. These two main tasks in the project have been undertaken in Work Packages (WPs) 2 and 4.

The way that PADAMOT activities fit into an overall scheme for increasing confidence in scenarios for safety cases by combined use of information about past climate and palaeohydrogeology is illustrated in Figure 1. The intermediate stages of the scheme involve interpretative models and expert judgements that transform proxy indicator data into the type of information that can be used in scenario development.

WP2 has produced data that characterise various types of solid media (secondary minerals, organic sediments, microfossils) as proxy indicators of palaeohydrogeology and geochemistry. Mineralogical and geochemical analyses have characterised fracture minerals from crystalline rocks, producing data that have been interpreted in terms of the relative timing of mineral formation and the geochemical conditions in groundwaters from which they precipitated. Analyses of organic geochemical, stable isotopic and microfossil proxy indicators of palaeoenvironment in Quaternary sediments have provided data for interpretation of climatic and hydrologic conditions at the times of sedimentation. Interpretation of these data in terms of understanding past evolution, quantifying processes and testing palaeohydrogeological models, is the development of models that simulate the proxy indicators. This modelling was undertaken in WP4.

WP4 has developed numerical models that provide links between the data and semi-quantitative information that have been obtained in WP2 and the features, events and processes (FEPs) that need to be considered in scenarios for long-term safety assessments. One of the models uses proxy data for climatic conditions to calibrate a hydrological model for the upper boundary of a groundwater system from which the variations of recharge are put into a time-dependent transport-reaction model to simulate how hydrogeological and geochemical conditions at repository depth change over time. Another model simulates how the deposition of fracture minerals might be related to changes of ambient groundwater conditions at depth which then leads to a quantitative model of the relationship between proxy indicator data in fracture minerals and hydrochemical conditions at the time of their deposition. The third model investigates how uncertainties in the conceptualisation and hydrogeological parameters for a fractured rock groundwater system affect interpretation of travel times and thus also affect the degree of confidence in the palaeohydrogeology of the system in response to changes at external boundaries.

The objectives of WP5 are: (i) to develop a methodology for incorporating palaeohydrogeological information in PA to demonstrate safety against long-term climate scenarios; (ii) to synthesise the outputs from the other WPs in PADAMOT, principally those from WP2 and WP4; and (iii) to evaluate the output from PADAMOT in terms of use for PA and to communicate these results and recommendations in a way that is usable by the PA teams.

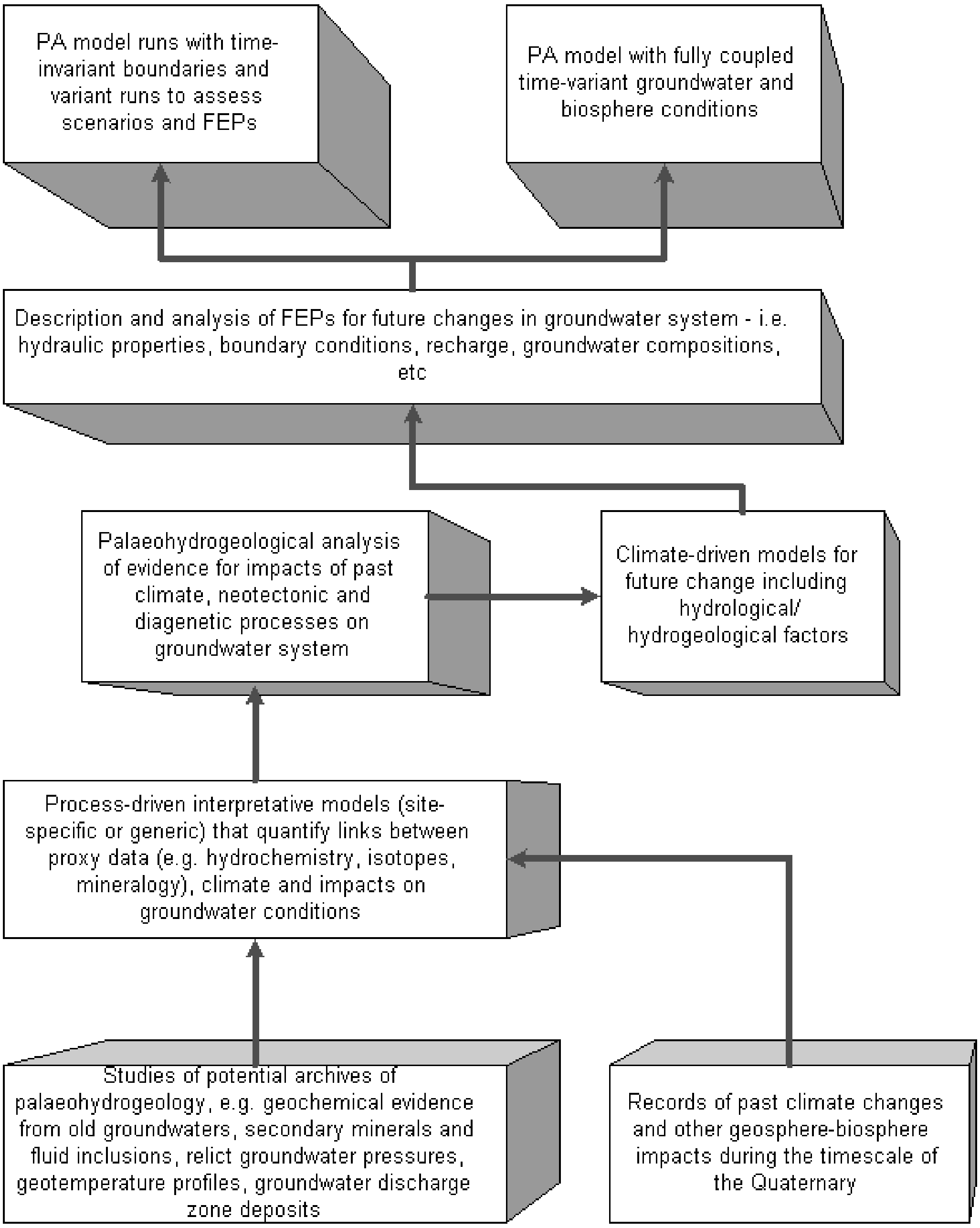


**Figure 1-1. Logical flow chart showing how palaeohydrogeological studies combine with independent records of past climate to provide data or qualitative information (e.g. FEPs) that feed in to various approaches to Performance Assessment (PA).**

## 1.2 SCOPE AND CONTENTS OF THIS REPORT

The contents of this report are as follows:

- Section 2 summarises a review of performance assessments that have been carried out so far on potential sites for deep repositories or as preliminary safety cases for typical repository systems. The review is reported in full in Appendix A. It focuses on the extent to which palaeohydrogeological information has been used, if at all, in the identification and constraint of scenarios for consideration in the safety cases. The purpose of the review is to find out to what extent the limited use of palaeohydrogeology so far in PA has been due to an assumption by PA teams of unchanging conditions or a restricted scope of scenarios and to what extent it has been due to the absence of palaeohydrogeological information that is usable in developing scenarios.

- Section 3 contains an analysis of the findings in Section 2 and then proposes a way of increasing the benefit of palaeohydrogeology to PA and of ensuring that information is not lost from a safety case. It suggests that all palaeohydrogeological information should be channelled into FEPs because these are the basis for scenario development. A subset of external FEPs, or 'EFEPs', are of particular relevance because these describe features, events and processes that might influence the geosphere of a repository system and therefore relate directly to palaeohydrogeology. A sequence of logical steps are proposed for producing palaeohydrogeological information from geochemical and mineralogical measurements and then for comparing this information with EFEPs.
- Section 4 describes and discusses the interpretations that are necessary to extract palaeohydrogeological information from geochemical and mineralogical measurements. An explanation of the scientific background illustrates the assumptions and the sources and magnitudes of uncertainties that are implicit in palaeohydrogeological interpretations. This should help PA groups to place appropriate degrees of confidence when palaeohydrogeological information is used for screening FEPs when scenarios are being considered. The section concludes by identifying two approaches to screening FEPs: one that focuses on specific lines of evidence and then links these qualitatively to FEPs, and a second approach that is a systematic screening of FEPs against palaeohydrogeological information. The first approach is used to make a conventional interpretation of PADAMOT data in Section 5. The second approach is described and, to a limited extent, illustrated in Section 6.
- Section 5 summarises the outcomes from WPs 2 and 4 in terms of information about palaeohydrogeology for each of the study sites. That information is then used to screen the validity and significance of certain EFEPs that might be significant for PA at the sites. Overall, two aspects of EFEPs are addressed: evidence for episodic changes of the movement and compositions of groundwaters over timescales in the past that are comparable with those in safety assessment, and evidence that the impacts of long-term climatic changes and other EFEPs on repository groundwater systems are attenuated with increasing depth.
- Section 6 develops and describes a structured approach to using palaeohydrogeological evidence for screening FEPs in safety cases. The methodology is know as Evidence Support Logic (ESL) and it assembles evidence from diverse sources, such as those contributing to palaeohydrogeological interpretation, and evaluates the strength of that evidence using a decision support model. For this application, ESL has the benefit of formalising and making transparent the subjective processes of expert judgement and the magnitude of associated uncertainties in drawing general conclusions from sparse or detailed data which has indirect significance to FEPs and safety cases. An application of ESL to palaeohydrogeological data and a safety case issue for one of the PADAMOT study sites illustrates the limitations of the approach when it is used in this way with the specific lines of evidence produced in PADAMOT rather than with all possible lines of evidence that are relevant to the scenario or safety case issue.
- Section 7 briefly draws some conclusions from WP5 and makes some recommendations about a methodology for incorporating palaeohydrogeological information into scenario development and PA and also about the implications for geochemical and mineralogical analyses and interpretations in site characterisation.

# 2 Palaeohydrogeological Information in Safety Cases

Palaeohydrogeological information is one of two main sources of evidence, the other one being natural analogues, that are available with which to test or moderate the degree of confidence in hydrogeological and geochemical aspects of a long-term safety case for a geological repository. There is therefore a strong requirement to carry out palaeohydrogeological studies of a potential repository site.

There are three main aspects of palaeohydrogeology for a potential repository site:

- Numerical modelling of hydrodynamics with parameters and boundary conditions that have been set according to expert judgement of past climate and other environmental impacts;
- Deductive interpretation and geochemical modelling of present-day groundwater chemical and isotopic compositions to deconvolute the 'signatures' of past infiltration conditions and the mixing of water masses that characterises past hydrodynamics;
- Characterisation and geochemical/isotopic analyses of secondary minerals and their fluid inclusions to obtain information about the groundwaters from which they were precipitated.

Palaeohydrogeological information from the interpretation of geochemical and mineralogical data is therefore the 'hard' evidence that tests and calibrates the validity of numerical models for the impacts of future changes of climate and other environmental variables on groundwaters. There is a need to develop robust, transparent and, as far as possible, quantitative ways of using that evidence to test the models, assumptions and scenarios that are used in Performance Assessment (PA). This major challenge - of improving the long-term credibility of PA - has been the issue that the PADAMOT project has set out to address.

A safety case must extend for many thousands of years and, for most regulatory frameworks, this is typically up to at least the timescale in which radionuclide releases might reach a maximum. Over that length of time, conditions at the surface will change due to climatic changes and conditions underground may change due to the downwards propagation of surface effects and also due to geologic changes. Conditions at depth where a geological repository would be located are generally less susceptible to change, benefiting from the inherent stability that rocks at moderate depths have in many locations. The lower susceptibility to disturbance and change is one major reason why geological disposal is the preferred option over storage at the surface for long-term waste containment. However that reduced susceptibility to change, and the degree to which a safety case depends on it, need to be tested and demonstrated in the natural geologic system if there is to be confidence in the models on which a safety case is based.

Performance assessments (PAs) up to the present time have generally simulated the long-term behaviour of a repository with numerical models that are parameterised for present-day conditions and that have assumed invariant conditions. The potential impacts on safety of environmental changes have been considered, if at all, by constructing alternative or variant scenarios representing possible future evolution. Alternatively, sensitivity calculations have been used to demonstrate that potential impacts of environmental changes lie within the range of uncertainty in the central or base scenario. Confidence in the validity of variant scenarios or sensitivity analyses, and in the implied overall stability of the deep geological environment, depends on independent evidence. Palaeohydrogeology and natural analogues are the two principal avenues of investigation for this type of evidence.

The climate-related scenario that is generally considered to have the greatest potential impact for those sites at northern latitudes is glaciation. Theory-based concepts of how groundwater conditions change under ice sheets and permafrost and how their potential impacts should be represented in base scenarios or variant scenarios have quite large uncertainties. These are areas where additional palaeohydrogeological information would improve the basis on which scenarios are developed for northern and central European regions that will experience glacial and/or periglacial conditions in the future.

Palaeohydrogeological evidence of the past impact of glaciation has been investigated most intensively by the programmes in Sweden, Finland, UK, Switzerland and Canada. Periglacial impacts (permafrost, meltwater run-off) have also been considered by the UK, Swedish, Finnish, Belgian and French programmes. In regions that are not susceptible to glaciation, the climatic and hydrological changes that are associated with global cycles of glacial and interglacial periods must still be considered in PA. This has been the case in Spanish and US programmes for which present-day regional climate conditions are semi-arid to arid.

Although climate-related changes in groundwater systems have been the focus of the PADAMOT project, other environmental or geological changes may also be of potential concern as variant scenarios over the timescale of PA. Palaeohydrogeological methods are equally applicable for obtaining evidence of past changes that will help to define and constrain scenarios in these cases. For example, uplift or subsidence due to plate tectonic processes is a significant, and perhaps dominant, cause of changes in the geosphere environment during a PA timescale for potential repository sites in Japan. In this case, a deep repository location does not necessarily have the simple benefit of stability that it has with respect to climatic impacts on groundwater, and thus methods for investigating palaeohydrogeology and past stability have great potential significance. Another case is the proposed repository at Yucca Mountain in the USA where the possibility of future hydrothermal activity within the PA timescale has been scrutinised closely by means of the palaeohydrogeological evidence for the existence, timing and intensity of past activity.

Twelve PAs are reviewed in Appendix A and the findings from this review are summarised in Table 2-1. Eight of these are for potential or generic repositories hosted in crystalline rocks: AECL 94 (Canada), SITE-94 and SR97 (Sweden), Kristallin-1 (Switzerland), Nirex 97 (UK), TILA 99 (Finland), H-12 (Japan) and AGP-Granite (Spain). Three PAs are for repositories hosted in clay rocks: AGP-Clay (Spain), SAFIR 2 (Belgium) and Opalinuston (Switzerland). A total system PA for site recommendation (TSPA-SR) was published in 2000 for Yucca Mountain (USA) for which the repository host is unsaturated volcanic rocks.

For many of the inland sites (AECL-94, Kristallin-1, Opalinus Clay, SAFIR-2, and Yucca Mountain TSPA-SR) palaeohydrogeological information has helped to define the reference scenario or base case used in PA. For coastal sites in the Fennoscandian Shield (SR-97, SITE-94 and TILA-99) palaeohydrogeological information has supplemented information about time-dependent changes due to land uplift and Baltic sea level change to build conceptual descriptions of base scenarios that incorporate evolution through glacial cycles.

In the Nirex 97, H-12 and AGP PAs, understanding of long term groundwater evolution in each case contributed to the development of conceptual models, but palaeohydrogeology was not used directly in the further development of numerical models because the base case groundwater model in each case assumed steady state groundwater systems with present-day boundary conditions.

It is apparent that palaeohydrogeology has been used variably in past PA exercises, from being virtually absent to having a major part in supporting models for both present-day conditions and impacts of past climatic episodes. To some extent this is due to the preliminary nature of many PAs carried out to date, in which the emphasis has been on evaluating safety for groundwater pathways as they are at present. Where variant groundwaters scenarios have been developed, the scope and impact of these on PA has been estimated and constrained usually by expert judgement. Evidence from site investigation to support or test such judgements has largely not yet been integrated into scenario development. In other words, the integration of site investigation data and modelling that underlies the base case for PA has not yet been extended to palaeohydrogeology and scenarios. As a result, uncertainties in scenarios might be unnecessarily high or unrealistically low.

Section 3 proposes an approach towards integrating palaeohydrogeology more consistently into PA. It suggests that this might be achieved by identifying the features, events and processes (FEPs) that could be better described and quantified by incorporating information from palaeohydrogeology. FEPs are the 'building blocks' of PAs and especially of scenarios, and are therefore the most appropriate and practicable interface between PA and palaeohydrogeology.

New developments in simulation codes and greater computing power are allowing PA calculations to take account of varying 'time-dependent' boundary conditions and system properties (as schematised in Figure 1-1). However the scope for sensitivity analyses is still limited by computing power especially considering the additional number of parameters for which sensitivity should be analysed in a time-dependent PA. Palaeohydrogeological information will be important in achieving a balance between practicality and realism.

For example, an ideal outcome of palaeohydrogeological investigations can be envisaged whereby they would show that climatic and other environmental changes over a relevant timescale in the past have not affected the host rock formation and groundwater system at repository depth at a particular site. A more likely outcome, as exemplified by PADAMOT studies, is that there are lines of evidence with varying weights that suggest some changes at repository depth, and in this case numerical simulations will be required to evaluate their significance for safety. The usual approach for sensitivity analyses has been to choose 'conservative' values for parameters that should result in an over-estimate of risk though the reliability and transparency of assumptions involved in this depend on the conceptualization of the system. Palaeohydrogeological methods, coupled with the development of robust quantitative interpretative models, will reduce the need for conservatism and improve the scientific understanding that underpins the conceptualization of time-dependent changes.

**Table 2-1. Summary of scenarios considered in PAs and of how palaeohydrogeology was interpreted and used directly in support of PA. Mod = Palaeohydrogeological numerical modelling; Chem = Interpretation of groundwater chemistry and isotope hydrology; Min = Interpretation of secondary minerals and fluid inclusions.**

| PA | Scenarios | Palaeohydrogeology | | | |
|---|---|---|---|---|---|
| | | Mod | Chem | Min | How was it used in PA? |
| Kristallin-1 | Alpine uplift is within uncertainty range of ref scenario; periglacial etc | ? | ✓ | × | Interpreted site data cited in support of geosphere stability for EBS performance |
| AECL-94 | None, $10^4$y timescale | ✓ | ✓ | ✓ | Supporting research and interpretation of site data |
| SITE-94 | Central scenario has EFEPs for permafrost, glaciation and sea level change | × | ✓ | × | Comprehensive review of palaeoclimate effects on geosphere including groundwaters |
| Nirex 97 | Steady state base case only | × | ✓ | ✓ | Comprehensive interpretation and modelling of site data in associated reports |
| SR97 | Land uplift in base scenario; climate scenario has effects of glaciation and permafrost on groundwaters | ✓ | ✓ | ✓ | Supporting research and interpretation of site data but not explicit in PA |
| TILA-99 | Various 'what if' scenarios incl. Glaciation, more fresh and more saline water, etc | ✓ | ✓ | ✓ | Used to constrain qualitative/semi-quant variants |
| H-12 | Seismicity, volcanism, uplift, erosion. No climate scenario | × | × | × | Palaeohydrogeology research not used in H-12; research recently started into possible climate effects. |
| AGP-Granite & AGP-Clay | Human intrusion and shaft seal failure were only scenarios | × | × | × | Research into impacts of climate change supported by palaeoclimate studies & palaeohydrology |
| SAFIR-2 | Normal evolution includes climate change, i.e. permafrost and glacial melt water effects | ✓ | ✓ | × | Base case supported by palaeohydrogeology; modelling with hydraulic gradients enhanced by melt water; review recommends support by multiple lines of reasoning including palaeohydrogeology |
| Opalinuston | Glacial loading, treated within sensitivity analyses of reference scenario | ✓ | ✓ | × | Base case supported by absence of perturbation shown by pore waters |
| YMP TSPA-SR | Nominal scenario qualitatively considers water table rise and variable infiltration flux over $10^4$-$10^6$y; qualitative extended climate model to $10^6$y; only igneous activity and human intrusion scenarios in full PA | ✓ | ✓ | ✓ | Supported by detailed site characterisation of secondary minerals, fluid inclusions, isotope hydrology and chloride mass balance |

# 3 Maximising the Value of Palaeohydrogeology in PA

## 3.1 INTRODUCTION: THE PROBLEM AND THE WAY FORWARD

It is evident from the review that there are several different reasons why palaeohydrogeology has been used so variably and mostly patchily in PA. Amongst these reasons are:

- Focus of preliminary PA is on steady-state modelling of the system as observed; scenarios are generally little developed, absent or consider only non-geosphere FEPs.
- Scenarios have been developed for 'worst case' conditions based on theoretical FEPs rather than realistic FEPs based on interpretations of site-specific information.
- Many PA models have been parameterised primarily with stochastic distributions of site-specific data or generic data, so that the general approach to PA modelling does not readily accommodate deterministic or interpreted palaeohydrogeological information with poorly constrained uncertainties.
- Palaeohydrogeological information, which contains variable and sometimes high degrees of uncertainty, is not expressed quantitatively as parameters that PA models can use.
- Palaeohydrogeology has mainly been considered in detail in the interpretation of site investigation data and is available in research reports as narratives.

With these reasons as starting points, a generic approach can be suggested for increasing the benefit that palaeohydrogeology can afford to PA, or at least for ensuring that information is not lost from the overall safety case.

It is recommended that information from palaeohydrogeology should be channelled into PA in the context of FEPs (Features, Events and Processes). FEPs offer a structure for considering potential time-dependent changes and impacts in a context of palaeohydrogeological evidence. A selection of FEPs from the International Database of FEPs (NEA, 1998, 2000) can be made that includes those that might be linked directly or indirectly with changes in groundwater conditions. These are set out in Table 3-1 which shows them arranged according to the structure of the database which creates a hierarchy of FEPs with the top-level categories identifying the source and type of time-varying influence on the system (note that EFEPs fall into one of these categories), intermediate categories representing the type of potential impact on groundwater conditions and solute transport, and individual FEPs describing the specific causes of impacts on groundwater conditions and solute transport pathways.

The hierarchy of FEPs has been changed slightly to focus the logic on evidence for palaeohydrogeological change that would support the inclusion of the associated FEPs in scenarios. Palaeohydrogeological change here includes variations in geochemical conditions as well as changes in past groundwater flow rates and directions.

The ways that the EFEPs can be developed into semi-quantitative or quantified scenario models are illustrated in Figure 3-1. This shows that 'external factor' FEPs (i.e. those concerned with geological and climatic changes) are considered for the specific site of interest, i.e. whether the site is coastal and what are the expected future climate states and climate-driven surface/hydrological processes. Bounding limits for these processes are then derived by research insights and these are applied to process models to estimate potential impacts on groundwater conditions at repository depth. These generalised process models might then be taken further to estimate specific impacts on flow rates, directions, travel times and compositions, though as the review has shown this level of detailed scenario development has not yet been widely realised in PAs.

**Table 3-1. External FEPs (EFEPs) for scenario development broken down into processes that use information from palaeohydrogeology (numbers are index numbers in The International FEP List; NEA, 2000). This scheme is also shown in Figure 3-1.**

| | Source and type of time-varying influence on system | Type of impact on groundwater conditions and solute transport | Specific cause of impacts on groundwater conditions and solute transport pathways |
|---|---|---|---|
| Assessment Basis (0): Timescales of Concern (0.02), Regulatory Requirements and Exclusions (0.09), Model and Data Issues (0.10) | External factors<br>Global climate change (1.3.01)<br>Regional and local climate change (1.3.02) | Hydrological/ hydrogeological response to geological change (1.2.10) | Tectonic movements and orogeny (1.2.01) |
| | | | Hydrothermal activity (1.2.06) |
| | | | Erosion and sedimentation (1.2.07)<br>Erosion and deposition (2.3.12) |
| | | | Diagenesis (1.2.08) |
| | | Hydrological/ hydrogeological response to climate changes (1.3.07) | Sea level change (1.3.03) |
| | | | Periglacial effects (1.3.04) |
| | | | Local glacial and ice sheet effects (1.3.05) |
| | | | Warm climate effects (tropical and desert) (1.3.06) |
| | Environmental factors in disposal system domain | Hydraulic/hydro-geological processes and conditions in geosphere (2.2.07) | Hydraulic/hydrogeological processes and conditions (2.2.07) |
| | | | Chemical/geochemical processes and conditions incl. pH and redox (2.2.08) |
| | | | Biological/biochemical processes and conditions (2.2.09) |
| | | | Hydrological regime and water balance (near-surface) (2.3.11) |
| | | | Mechanical processes and conditions (2.2.06) |
| | Factors affecting radionuclides | Radionuclide release and migration in geosphere pathways | Speciation and solubility enhancement (3.2.02) |
| | | | Sorption/desorption processes (3.2.03) |
| | | | Chemical/complexing agents, effects on speciation and transport (3.2.05) |
| | | | Microbiologically-mediated processes (3.2.06) |
| | | | Water-mediated transport (3.2.07) |
| | | | Gas-mediated transport (3.2.08) |
| | | | Interactions and transport with colloids (3.2.04) |

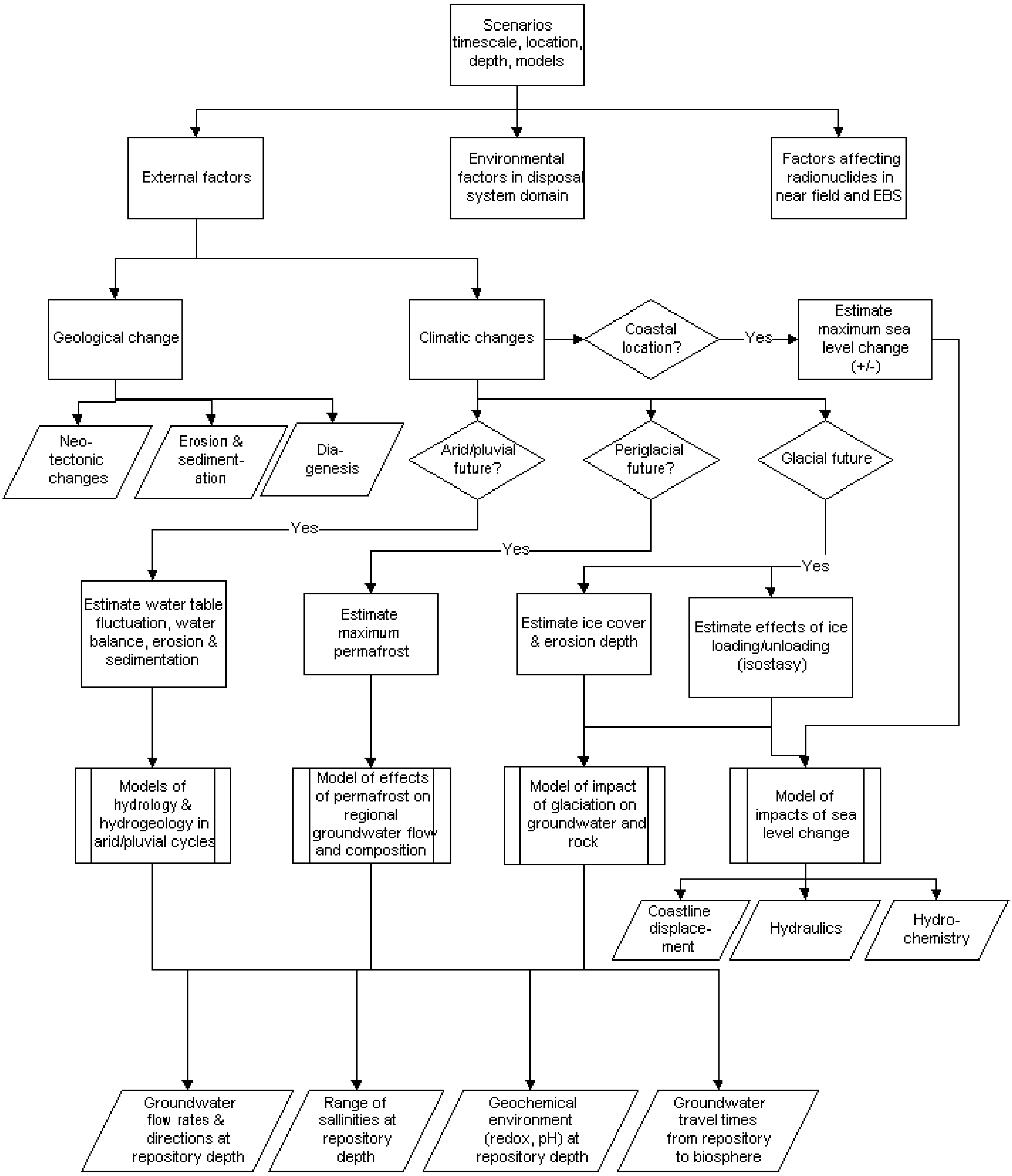


**Figure 3-1. Flow chart showing how scenarios are described in terms of EFEPs (in rectangular boxes) that can be linked with palaeohydrogeological information and other palaeoindicators (in diamond-shaped boxes) via interpretative models (rectangular boxes with double sides).**

## 3.2 DETAILS OF THE PROPOSED METHOD

The proposed method for considering palaeohydrogeology in PA comprises several interpretative and assessment steps. These will evaluate palaeohydrogeological information in the specific contexts of PA requirements and of scientific knowledge and models. Quantitative data or qualitative information will be the outputs from geochemical and mineralogical methods and will provide varying degrees of constraints on the past impacts of EFEPs. This information will, preferably, be placed in a chronology that enables it to be linked to the known timescales of climate-driven EFEPs and boundary conditions. The interpretative steps between geochemical and hydrogeological measurements and inferred palaeohydrogeological information are illustrated in a flow chart in Figure 3-2:

A. Geochemical and hydrogeological data are obtained by measurements at the site of interest. These will include:

- Groundwater chemistry: Compositions of deep groundwaters are likely to comprise mixtures of components of different origins and ages that contain information of pre-existing conditions, and the mixing process also contains information about past hydrodynamics.
- Isotope hydrology: Stable isotopic ratios are indicative of origins and palaeoclimatic conditions for meteoric waters, and cosmogenic and nucleogenic nuclides ($^{14}C$, $^{36}Cl$, etc) relate to groundwater ages and solute residence times.
- Minerals assemblage: Secondary minerals are relicts of pre-existing alteration reactions and groundwater compositions.
- Mineral geochemistry, morphology and zoning: The bulk geochemical compositions of secondary minerals are indicative of the gross chemical environment at the time of formation and may be amenable to geochemical modelling to obtain semi-quantitative limits on e.g. redox, pH, carbonate; growth zones, sometimes associated with fluid inclusions may have developed, allowing a relative chronology to be placed on the evolution of past geochemical conditions.
- Mineral isotope compositions – stable C and O isotopic compositions of carbonate minerals relate to the groundwater compositions from which they formed, the temperature, and possibly also the prevalence of microbial activity and origins of carbon (e.g. soil development at the time of recharge); U and Th isotopes may indicate age of secondary mineral growth and subsequent mobilisation of U due to varying geochemical conditions.
- Groundwater pressures – these may indicate the existence of transient head conditions that are relicts of palaeohydrogeological boundary conditions for the groundwater system (this is not considered further here).

B. Geochemical and mineralogical data have to be interpreted to produce information about past groundwater conditions. Interpretative methods vary from quantitative geochemical models to qualitative expert judgement:

- Groundwater chemical compositions and stable isotope ratios are interpreted to obtain information about the component water origins by graphical techniques, reaction-mixing modelling and statistical modelling.
- Isotopic data related to water ages are interpreted by calculations that involve estimates or assumptions about initial compositions ($A_o$ at $t = 0$), dilution due to water-rock reactions, and in situ production of isotopes.
- Minerals assemblage (i.e. paragenesis) data are interpreted by expert judgement of the environment in which the minerals are stable.
- Geochemical compositions of bulk minerals and of individual growth zones are interpreted semi-quantitatively by stability diagrams or by other methods that relate mineral composition to co-existing solution composition.
- Isotopic compositions of minerals are interpreted for stable isotope fractionation to obtain co-existing groundwater compositions; U-Th data are interpreted to obtain mineral ages by parent-daughter isotope system calculations for which various assumptions are necessary.

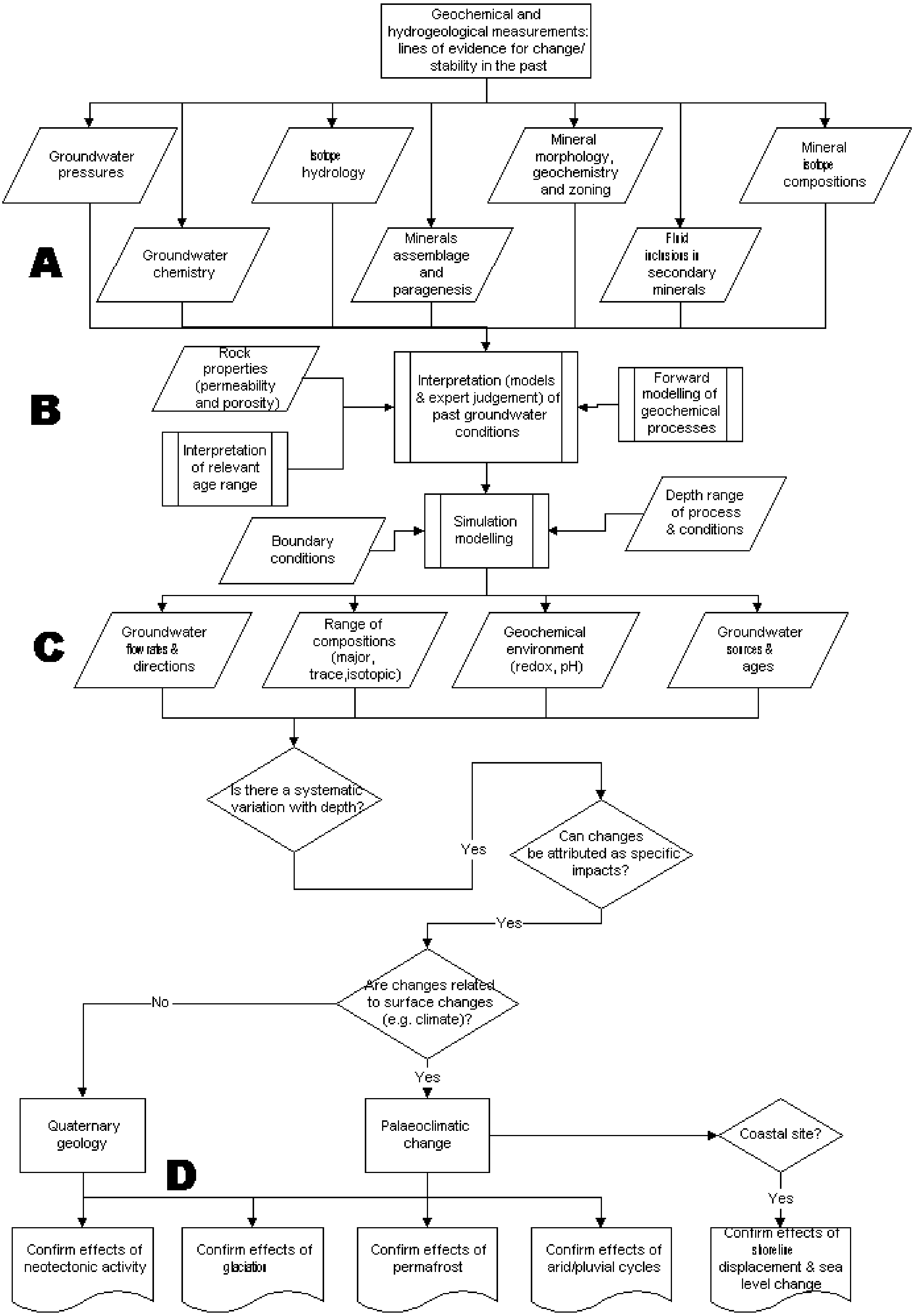


**Figure 3-2. The interpretative steps that produce palaeohydrogeological information from hydrochemical, geochemical and mineralogical measurements. It shows that there are two stages at which a comparison of information with that produced in PA scenarios is possible: at stages C and D.**

It is important to recognise that these interpretations are likely to produce rather disaggregated palaeohydrogeological information that relates to limited spatial and temporal intervals. They are unlikely to produce a coherent and detailed model of evolution of the whole groundwater system over the timescale of interest – the integration of the various bits of information is an interpretative task in which expert judgement inevitably has an important role. In general, interpretation of groundwater data (chemistry and isotopes) identifies the major water components in terms of their typical compositions, sources and ages. Interpretation of minerals data relates to localised geochemical conditions during a discrete interval of mineral growth (or several intervals that may or may not be contiguous). There are many sources of uncertainties in the interpretations of geochemical conditions, of time intervals for which the evidence applies, of the spatial variability, and of the relationships to groundwater movements. Expert judgement is necessary to assess the uncertainties and to consider the possibilities for alternative models. Forward modelling of geochemical processes from hypothetical or typical starting conditions may be valuable as a simplified simulation of the evolution of the real system.

C. The resulting palaeohydrogeological information can be divided into five categories:

- groundwater flow rates and directions in the past (though direct evidence of this is rare);
- ranges of salinities in the past;
- geochemical environment, especially with respect to pH and redox;
- groundwater sources and ages, solute residence times;
- degrees of groundwater mixing.

This information may be directly comparable with the outputs from hydrogeological and geochemical models that are used in developing PA scenarios (see next section and Figure 3-2). This is a basis for using palaeohydrogeological information as a way of testing whether the system variability introduced by scenario analysis is appropriate for that particular site.

D. Another basis for comparing palaeohydrogeological information with the scenarios used in PA is examination of evidence for the impacts of palaeoclimatic events. This involves some additional stages of interpretation and combines the various types of interpreted data to support generalised 'expert assessment' of the impacts of past climate episodes. Thus more expert judgement is involved in this approach. It is also desirable to have chronological information because knowledge of global palaeoclimate already has a good chronology and correlation of climate-driven changes at the surface boundary with changes within a groundwater system plays an important part in this approach. It has a possible advantage in shifting the basis for comparison back one stage in the modelling of scenarios which is more realistic in terms of how scenarios have been developed in recent PAs. Essentially, this additional step in interpretation puts the onus on the palaeohydrogeological investigations to achieve a chronology of change that can be correlated with the chronology of past climate change and of consequent changes in boundary conditions.

In addition to the direct (i.e. hydraulic) propagation of palaeoclimatic changes into the groundwater system, geological effects during the Quaternary period might also have changed groundwater conditions. For example, crustal depression or tilting due to glacial loading could also have perturbed the water table and fresh-saline water interfaces. Given some degree of geochronological information about discrete episodes of physical or chemical processes (e.g. U-Th dates of secondary carbonate, $^{14}C$ or $^{36}Cl$ ages of groundwater components), it might be possible to interpret groundwater changes as directly linked to those episodes:

- Glaciation – injection of meltwater below warm-based ice sheets or from periglacial ice lakes. Geochronology should correlate with a period of glacial advance or retreat.
- Permafrost – reduction of general infiltration and recharge, localisation of discharge, possible salination of shallow groundwater. Geochronology should correlate with prolonged periods of periglacial conditions prior to glacial maxima.
- Arid/pluvial cycles – large fluctuations of recharge and of water table position in southern and central Europe regions. Geochronology may correlate approximately with glacial periods experienced in northern Europe. Processes with datable indicators may include deep oxidative weathering, secondary mineralisation at water table, episodic salinization, evaporite minerals.
- Sea-level change and shoreline displacement - intrusion of marine water into coastal aquifers, secondary mineral precipitation and/or karstification in mixing zone.
- Neotectonic activity – reactivation of faults and precipitation of secondary minerals, movement of fresh/saline groundwaters and interfaces (in reality, these processes are probably indistinguishable from other processes driven by climate factors).

# 4 Information for EFEPs from Interpreted Geochemical and Mineralogical Data

This section of the report describes and discusses the scientific interpretations that are necessary to extract palaeohydrogeological information from geochemical and mineralogical measurements. Valuable data is obtained from groundwater and mineral samples, and this report focuses on data from minerals because that was the priority of PADAMOT. An explanation of the scientific background with a consideration of the degrees of uncertainty should assist PA groups in placing appropriate degrees of confidence in palaeohydrogeological information for 'screening' FEPs and scenarios. There are essentially two approaches to screening: (i) a qualitative judgment of the significance of palaeohydrogeological information, and (ii) a structured examination of the evidence from palaeohydrogeology in the context of particular FEPs and impacts on the groundwater systems. The second approach will be described in Section 6 with an example of its application to FEPs contributing to a climate-change scenario for a PA exercise.

## 4.1 SCIENTIFIC BACKGROUND RELATING GEOCHEMICAL AND MINERAL DATA TO EFEPS

### 4.1.1 Mineral paragenesis

Minerals paragenesis refers here specifically to the suite of secondary mineral reactions (i.e. precipitations and dissolutions) that have occurred in the groundwater-rock system of interest. For present purposes, the paragenesis can be restricted to a relevant timescale although older stages of the paragenesis might have a role in dissolution reactions and buffering of geochemical conditions.

Secondary minerals that are thought to have formed in the relevant timescale, i.e. that of the Quaternary period which is about the last two million years, are referred to here as 'late stage'. Late-stage minerals are typically calcite, clays and iron oxides. The presence or absence of these minerals, and their abundances, distributions and relationships, characterise groundwater composition and water-rock reactions when they were precipitated. Geochemical and mass transport modelling in Work Package 4 has illustrated some of the processes in shallow and deep fractured rock environments. In the case of the Ratones research site, the chemical compositions of groundwaters in the faulted zone of high transmissivity are deduced to change as the recharge rate varies with climate. These changes in turn affect the paragenesis of late-stage minerals:

- dissolution of ankerite and calcite,
- oxidation of iron sulphide and precipitation of iron oxide,
- dissolution and precipitation of apatite,
- alteration of albite plagioclase to clay minerals.

Dissolution of the carbonate minerals is indicative of groundwater conditions with higher $Pco_2$ and lower pH than in locations where the calcite precipitates. Oxidation of Fe sulphide and precipitation of Fe oxide are indicative of more oxidising conditions relative to those in which uncorroded Fe sulphide is preserved.

Modelling in WP4 suggests that relatively less oxidising conditions in the Ratones groundwaters is associated with lower recharge, i.e. more arid conditions. The reactive transport modelling also shows that the mineral paragenetic changes, i.e. amounts of minerals and response to geochemical changes, are likely to be much more marked in a transmissive fault than elsewhere in the bulk rock mass.

### 4.1.2 Mineral morphologies

The morphology, or crystal shape, of a secondary mineral may indicate some dependence on the hydrochemical environment in which the crystal grew. Morphology of the surface layer may relate to ongoing growth at the present day; changing morphologies of successive growth layers indicate that chemical conditions changed over the period of growth. Solute ions that are known to influence growth rates on contrasting crystal faces, and thus morphology, of calcite are Mg and other trace components such as Sr, Mn and Fe. Variations in the concentration of Mg relative to Ca are most marked between fresh and saline waters. Indeed, morphology of secondary calcite is well established as an indicator of salinity (Milodowski et al., 1997). For example, a morphological transition is found in secondary calcite at the Sellafield site that corresponds to a groundwater salinity transition from brackish to saline.

Past changes of salinity are of intrinsic interest as EFEPs and also suggest hydrodynamic changes. Variations of groundwater compositions, and mixing within groundwater systems with varying salinity, have been shown in WP4 modelling to be probably the major cause of secondary calcite precipitation in deep groundwaters.

### 4.1.3 Compositional variations in growth zones

Variations of composition of growth zones in secondary calcite reflect changes in groundwater compositions. The growth zones are initially detected during petrographic examination of secondary minerals as alternating light and dark bands of cathodoluminescence (CL). The patterns of CL banding in secondary calcite vary systematically through a site, as at Sellafield, suggesting that they relate to spatial and temporal variations of groundwater composition. Chemical compositions of CL zoning have been investigated with electron microprobe and ion probe analyses in WP2, showing that zoning correlates with variations of Fe, Mn, Mg and other trace element contents. Of particular interest are the variations of redox-sensitive trace elements, namely Fe, Mn and Ce, which suggest that the CL zoning is a palaeohydrogeological 'archive' of past redox conditions. Making the assumption that Fe:Mn ratios in secondary calcite are the same as those in the parent groundwater at the time of precipitation, geochemical modelling has been used in WP4 to study the implications of these Fe and Mn variations in calcite zones for redox variability. WP4 modelling confirms that high Fe:Mn ratios, correlating with dull CL banding, generally correspond to more reducing conditions, whilst low Fe:Mn, correlating with bright CL banding, correspond to less reducing conditions. However the modelling also shows that these are possibilities of alternative interpretations of Fe:Mn ratios in terms of redox. Distinguishing between these alternative models requires knowledge of the Fe- and Mn-containing mineral phases that control solution compositions during the precipitation of calcite. Ca variations between the CL zones have been detected by ion microprobe in WP2 and can similarly be related to redox variations.

### 4.1.4 Mineral dissolution fabrics

Evidence of mineral dissolution in the fabric of secondary mineralisation and of primary wallrock minerals is a more subtle indicator of palaeohydrogeological conditions. This is because it involves interpretation of what is missing – what has been removed. Dissolution, i.e. under saturation of groundwater compositions with respect to a particular mineral that has been present, indicates that geochemical conditions changed. For example, studies of drillcore samples from Sellafield in WP2 have suggested that anhydrite, $CaSO_4$, has been removed. This is interpreted as indicating a switch of groundwater composition from saline/brine, in which $CaSO_4$ is saturated, to less saline, in which $CaSO_4$ is undersaturated and thus destabilises a pre-existing anhydrite paragenesis. Dissolution fabrics may also be detected micropetrographically at the boundaries between growth zones in calcite, suggesting that groundwater compositions and hydrodynamic mixing may have fluctuated so that the state of calcite equilibrium has fluctuated either side of saturation.

### 4.1.5 Stable isotopic (O and C) compositions

Stable isotope ratios, $^{18}O/^{16}O$ and $^{13}C/^{12}C$, in secondary calcites have been measured in WP2 by a number of techniques and at various scales of resolution. $^{18}O/^{16}O$ of calcite is controlled primarily by the $^{18}O/^{16}O$ and the temperature of co-existing water from which calcite precipitation occurred. $^{18}O/^{16}O$ in calcite, specifically in discrete growth zones, is therefore potentially an important palaeohydrogeological indicator. By making reasonable assumptions about the probable maximum deviations of past geotemperatures in deep groundwaters from present conditions, $^{18}O/^{16}O$ data have been interpreted in WP2 as strong evidence for significant proportions of glacial melt water to have penetrated to considerable depth at Sellafield in the past, presumably corresponding to a glaciation episode. $^{13}C/^{13}C$ in calcite reflects the $^{13}C/^{13}C$ of dissolved inorganic carbon (DIC) in groundwater at the time of precipitation. $^{13}C/^{13}C$ of DIC is controlled by the sources of carbon, specifically the proportions of atmospheric $CO_2$, dissolved carbonate mineral, and organic C from superficial soils or other organic sources that have been mineralised by microbial respiration. $^{13}C/^{13}C$ variations in secondary calcite therefore indicate fluctuations in sources of carbon that may relate to changing climate impacts at the surface, e.g. varying degrees of soil development, and/or to changing microbial activity or carbon sources in deep groundwaters.

### 4.1.6 Fluid inclusions

Fluid inclusions are microscopic volumes of groundwater or other fluids (e.g. gases, hydrocarbons) that have been trapped in secondary minerals (usually quartz or calcite) as they grew. They are the most direct palaeohydrogeological indicators but, considering analytical limitations and also their chemical stability for preserving redox-sensitive compositions, they effectively provide data on past salinities and possibly stable isotopic compositions. Temperatures may also be inferred from experimental homogenisation of two-phase inclusions.

### 4.1.7 Mineral dating

It is obviously important to obtain, if possible, absolute ages for secondary calcites that puts the timing of their formation into the geological timescale. In the present context and application for palaeohydrogeology, the timescale of interest is comparable with the timescale over which a repository safety case needs to be projected into the future, i.e. up to a million years. Thus 'late-stage' calcites in this study are assumed to have been precipitated during the Quaternary period and thus to be the product of groundwater regimes through the alternating glacial and interglacial climatic episodes of that period. Isotopic analyses that could potentially be relevant to this timescale are the U-Th system and carbon-14. Decay of $^{234}U$ to $^{230}Th$ has a half life of $2.45 \times 10^5$ years, so this system is of greatest potential interest. However all of the secondary calcite samples in this study have concentrations of U that are too low for meaningful analyses by presently-available techniques, especially when considering that the ages of individual growth zones are ideally needed. $^{14}C$ has a decay half life of $5.73 \times 10^3$ years and would therefore be of potential value for the youngest generations of late-stage calcite only. However the $^{14}C$ evolution of inorganic carbon in groundwaters involves substantial dilution of atmospheric C inputs due to dissolution of mineral carbonate, so the $^{14}C$ content of even the youngest secondary calcite is extremely low and is effectively uninterpretable in terms of age of formation of the calcite.

### 4.1.8 Present-day groundwater compositions and age data

PADAMOT has been concerned primarily with palaeohydrogeological information from secondary minerals, but that cannot be isolated from the information that can be obtained from interpretation of the 'palaeowater' components that are relict in present-day groundwaters. Preliminary data from the Melechov site are reported in WP2, and groundwater compositions, including comprehensive isotopic data, have previously been reported for the Sellafield, Äspö and Ratones sites (Bath et al., 2005; Laaksoharju et al., 1999; Gómez, 2002). Interpretation of hydrochemical and isotopic data for deep groundwaters usually requires the deconvolution of mixtures to obtain information on the water sources and chemical processes that are of palaeohydrogeological significance. For example, interpreted groundwater ages and/or solute residence times may reveal inconsistencies with present-day hydrodynamics, suggesting that groundwater flow rates and boundary conditions have changed over time in response to EFEPs.

## 4.2 UNCERTAINTY AND ASSUMPTIONS

It is clear that there are many sources of uncertainty in how geochemical and mineralogical data are related to information on EFEPs. Uncertainties in palaeohydrogeological interpretation can be categorised broadly into those originating in data and those associated with interpretations. If palaeohydrogeological information is to be used to describe EFEPs and to construct scenarios for PA, then the uncertainties and probability of occurrence should be clear for the users. The following paragraphs describe where there are significant uncertainties in using palaeohydrogeological information for EFEPs and scenarios.

### 4.2.1 Uncertainty in geochemical and mineralogical data

In general, the uncertainties in geochemical and mineralogical analyses are likely to be less significant than those in interpretations.

Identification and descriptions of minerals, mineral parageneses and growth features are reliable if based on observations by an experienced petrographer using micrographic instrumentation. A large number of micrographic measurements are needed to interpolate observations through a rock volume typical of a repository site and to identify spatial patterns with reasonable reliability. Incompleteness of data is therefore likely to be the dominant source of uncertainty in the interpretation of mineralogical information. Uncertainties in the descriptions of secondary mineral assemblages and parageneses become most significant if trace accessory minerals are missed or wrongly identified. Minerals that influence the interpretation of palaeoredox, as illustrated by geochemical modelling of Fe and Mn variability in WP4, are important in this respect. For example, presence or absence of pyrite, iron oxide or siderite co-existing with calcite is a significant observation, as illustrated in WP2.

The late-stage mineral parageneses have relative ages attributed according to their growth characteristics. Generalised ages for formation in the geologically-recent past, e.g. 'Quaternary', have been estimated on the basis of petrographic judgment. In the present study it has not been possible to measure geochronological isotopes, i.e. the U-Th system, so calibrated absolute ages are not available. The only geochronological isotopic data are four earlier U-Th ages on bulk late-stage fracture calcite from Sellafield giving ages up to 370 ka with rather high uncertainties (Nirex, 1997). Relatively light stable oxygen isotopic ratios ($^{18}O/^{16}O$) of secondary calcites are inferred to originate from isotopically light 'cold climate' groundwater and thus to indicate Quaternary age, i.e. that these calcites formed at some time in the last 2 million years. In summary, there are significant uncertainties in the ages of the late-stage secondary mineral parageneses – it is probable that they represent growth during the Quaternary, i.e. in the past timescale of interest, but this is not confirmed. Isotopic compositions of secondary calcites and of growth zones within calcites that are light relative to equilibrium with present-day water are reasonably interpreted as having precipitated from cold-climate waters. It is uncertain in each case whether these cold-climate isotopic signatures date from the most recent glaciation (i.e. around 20 ka) or from preceding glacial episodes up to 2 million years ago.

One of the most significant sources of uncertainty in geochemical analyses of secondary minerals is the variability of compositions within and between growth zones. This variability has been demonstrated by the combined application of instrumental microanalytical techniques (CL, EPMA, SEM-EDXA, LACE-ICPMS, ion probe) to secondary calcites in WP2. There are variations in trace element contents and stable isotopic compositions that match roughly with scales of growth zoning as identified by CL, but it is not clear that there is an exact correlation. Knowledge of this variability raises several issues. Firstly, is the question of how it relates to temporal fluctuations in groundwater compositions – in modelling of Fe and Mn variations in WP4, it has been assumed that there is a direct relationship. Secondly is the question it raises about the value of 'averaged' analyses on bulked samples from across several growth zones – this uncertainty applies to various trace element and stable isotope data sets in WP2 for which some caution is necessary with detailed interpretations although the 'averaged' analyses retain considerable value. A general aspect of uncertainty is that application of microanalytical and micrographic techniques inevitably results in the detection of increasing complexity in compositional variations at smaller scales. There are, as yet, few natural systems or experiments in which the hydrogeochemical significance of microscopic compositional variations in actively-growing mineral precipitates has been studied.

An uncertainty that is associated with compositional variations and the development of distinct growth zones is the extent, if any, of re-equilibration of older mineral growth material with more recent groundwater. Interpretation assumes that re-equilibration does not occur and there is considerable evidence, for example the distinct boundaries between growth zones, that support the assumption. Bulk re-equilibration is clearly discounted by the existence of compositionally-distinct growth zones.

Analyses of fluid inclusions to derive temperatures of formation, salinities and concentrations of specific solutes (e.g. by LACE-ICPMS analyses) have uncertainties that may be relatively large. Salinity of inclusions is estimated from freezing temperature, $T_{ice}$, and the lower limit of quantification is brackish/saline, so this method does not distinguish fresh from brackish inclusion fluid. There is also a lower limit on temperature estimation because low temperature inclusions, i.e. those of direct interest for palaeohydrogeology, tend to be monophase. These uncertainties, plus relatively large uncertainty generally in salinity and temperature estimations and in calibration of solute analyses by LACE-ICPMS, are implicitly in the results of fluid inclusion studies in WP2.

### 4.2.2 Uncertainty in palaeohydrogeological interpretation

Interpretative models (conceptual and/or numerical) are invariably involved in the palaeohydrogeological interpretation of indicator data. The types of models are exemplified as:

- Geochemical equilibrium models of water-rock reaction;
- Hydrochemical mixing models;
- Hydrological water balance models relating climate variables with groundwater recharge;
- Groundwater flow and mass transport-reaction models to simulate effects of changing hydrogeological and/or geochemical initial and boundary conditions;
- Isotopic fractionation factors;
- Calculation of groundwater ages from isotopic data.

Geochemical equilibrium models are the basis for interpretations that particular minerals or mineral assemblages are indicators of specific hydrogeochemical conditions, e.g. Fe oxide occurrence is equated with oxidising conditions and pyrite, $FeS_2$, is equated with reducing conditions. These may be oversimplistic interpretations and more rigourous interpretations can be achieved by using geochemical speciation and equilibrium calculations to test equilibria for specific water compositions and mineral phases. This approach has been used in WP4 to evaluate the relationships between Fe and Mn concentrations, mineral assemblage and redox conditions. The main source of uncertainty in the use of a geochemical model is the initial conceptual model, i.e. the mineral equilibria and solution species that are included, and the assumption concerning water-mineral equilibrium. The assumption of local equilibrium being achieved by water-mineral reactions often has uncertain validity but is usually used because of the uncertainties in parameterising reaction kinetics. Thermodynamic data, especially for complex mineral phases, may also be a source of uncertainty.

Hydrological water balance modelling is a particularly significant aspect of palaeohydrogeology in arid climate conditions. This type of model, as demonstrated in WP4, relates recharge rate, i.e. the upper boundary condition of a palaeohydrogeological model, with palaeoclimate. Uncertainty in estimated recharge rates derives from the models for climatic dependence of evapotranspiration and run-off. That uncertainty is propagated into palaeohydrogeological model simulations of water table position, hydraulic gradients and flow rates. The net effect on the parameters for the EFEPs of a groundwater system is illustrated by calculations in WP4.

Coupled models of groundwater flow, mass transport and geochemical reaction illustrate how uncertainties in both hydrological and geochemical parameters are propagated into palaeohydrogeological simulations of hydrochemical evolution and precipitation of secondary minerals. $CORE^{2D}$ modelling in WP4 shows how hydrogeochemistry and hydrogeology are coupled in the system at Ratones, illustrating that spatial variations of geochemical and mineralogical indicators are dependent on the flow regime, so that variability in the later will have influenced the former. PRECIP modelling of secondary calcite growth in a mixing saline groundwater system as at Sellafield reaches similar conclusions.

Stable isotopic ($^{18}O/^{16}O$) fractionation has been used as a palaeohydrogeological indicator of groundwater origins in WP2 studies at Sellafield. Oxygen isotopic fractionation between water and secondary calcite is also a function of temperature, and this dependence introduces significant uncertainty into interpretation of the isotope ratio in terms of groundwater origin and age.

Uncertainty in the model interpretation of groundwater ages from isotopic data ($^{14}C$, $^{36}Cl$, etc) derives from a number of assumptions that have to made about initial isotope abundances and subsequent geochemical and physical processes that might have reduced (or enhanced) the isotope concentration in parallel with radioactive decay. Except in special circumstances in which the parameterisation of the interpretative model is particularly reliable, the uncertainty range in groundwater ages is likely to be between 0.5 to 5 times lower or higher respectively than the 'most likely' estimate, tending towards greater uncertainty at lower isotope abundances, i.e. higher ages. The complexity of dispersive groundwater mixing as age increases means that interpreted isotopic 'ages' have more complex hydrodynamic significance in terms of alternative hydrogeological models.

## 4.3 SCREENING METHODS FOR EFEPS USING PALAEOHYDROGEOLOGICAL INFORMATION

The preceding paragraphs discuss the scientific background that relates EFEPs to palaeohydrogeological interpretations of geochemical and mineralogical data, and the associated uncertainties. It is clear that there is a large dependence on interpretative modelling and expert judgment. The next step in using palaeohydrogeological information for PA is to consider what approaches might be used to assess the validity and potential significance of EFEPs in scenarios for PA against that information. Two basic approaches are considered here: firstly the procedure of interpreting geochemical and mineralogical data, preferably using quantitative models or calibrations, and then using expert judgment to draw conclusions of relevance to EFEPs from each individual line of evidence. For example, the data obtained in WP2 lead to inferences about past changes, or conversely about stability, in salinity, redox and other aspects of the hydrochemical environment. This is the procedure that has been used in past instances of using palaeohydrogeology in support of PA, as described in Section 1.

A second approach is a more systematic ‘screening’ of EFEPs against palaeohydrogeological information using a formal method for evaluating and weighting evidence. Evidence Support Logic (ESL) is a procedure for doing this. A small pilot study has used ESL to assess the proposition that ‘climate-driven changes over the Quaternary have had little impact at repository depth’, using the subset of palaeohydrogeological information for Sellafield in WP2.

The first approach is presented in Section 5 as a summary of interpretations and discussion of PADAMOT data. The second approach is described in Section 6.

# 5 Support for FEPs from Palaeohydrogeological Information

In this section of the report for Work Package 5 of PADAMOT, the information about palaeohydrogeology from WPs 2 and 4 will be used to screen the validity and significance of external FEPs (EFEPs) that influence PA. As discussed in the preceding section, there are two suggested approaches to this of which the first approach, using interpretation and judgement of specific information, is used here. The second approach, structured evaluation of evidence using ESL, is illustrated in the next section.

Interpretation and judgement of the geochemical and mineralogical data from WP2, and of the modelling in WP4, will be focused on two key questions that are of direct importance in screening EFEPs for PA:

- What changes, that are not a simple extrapolation over time of what is observed in the present-day groundwater system, affect groundwater compositions and movements over a timescale comparable with the assessment timescale?
- To what degree is the impact on the groundwater system of long-term environmental changes at the surface attenuated with increasing depth?

Palaeohydrogeological information from each of the PADAMOT research sites will be evaluated against these questions.

## 5.1 LOS RATONES AND PADUL/CÚLLAR-BAZA, SPAIN

### 5.1.1 Background

The main objective of palaeohydrogeological research at the Los Ratones Uranium Mine site was to study the impact of past environmental conditions at the theoretical depth in granite of a high-level waste repository. It is located in the Albalá granitic pluton in the southwest of Spain which has experienced fluctuating aridity and water table elevation in the past. The specific objective for PADAMOT studies was to obtain site-specific data on shallow and deep fracture-filling minerals which could potentially provide a record of the groundwater evolution in this area. Hydrochemical and minerals data have been used for palaeohydrogeological interpretation and modelling.

The strategy followed was:

- To analyse the composition of deep subsurface waters flowing through fractures because of the potential information that it can provide on the geochemical and hydrological evolution of the system. In particular, this could provide an understanding of the major chemical processes which control water composition flowing through fractures in this area.
- To determine the mineralogical and chemical composition of secondary minerals, including fracture-fillings, and to determine their spatial distribution and relationship with groundwaters. Special emphasis has been placed on characterising the carbonate minerals in the system.

Five boreholes were drilled around the mine to depths of up to 500 m. Borehole SR-1 is inclined and cuts dyke 27 between 65 and 75 m in depth. Borehole SR-2 (79 m deep) sampled waters that circulate through the Northern Fault at a depth of 58-60 m; these waters are considered to represent the recharge waters flowing into the mine. Borehole SR-3 (195 m deep) sampled groundwaters that flow at a greater depth through the Northern Fault (140-150 m), and enabled information to be gained on the chemical evolution of the water as a function of depth, between two hydraulically connected zones. Borehole SR-4 (124 m deep), located at the southern part of the mine sampled waters from the Southern Fault, which according to the hydrogeological conceptual model of the zone, would have been a previous pathway for the water discharge from the mine. Borehole SR-5 (500 m deep) is located to the south of the mine but is far away from the dykes. The chemical composition of the waters from this borehole reflects the impact of the mine on the deep granitic groundwater.

Three hydrogeological units can be distinguished:

(a) Areas of superficial cover characterized by short and shallow flows and seasonal springs, and that can constitute part of the recharge and subterranean discharge of the granites.

(b) Altered and fractured zones (150-200 m depth) characterized by relatively high transmissivities. The main structures and the network of minor fracturing connecting with them control the flow.

(c) Fresh granite that constitutes a low permeability media, in which the water flows through fractures. The flow is preferentially through the NE-SW fractures and the mineralized dykes (27 and 27').

The flow is controlled by the topography to a depth of at least 200 m. Below this depth the flows are regional and originated away from the influence of the mine. The most important water-rock interaction process with respect to the neutralization of pH in those waters affected by sulphide oxidation is the dissolution of carbonate minerals found in the fractures and dykes. Furthermore, the precipitation of siderite has a significant contribution in the regulation of $Fe^{2+}$ and $HCO_3^-$ in the mine waters. Ionic exchange with smectites in the fissure fillings is the main process that controls the cation concentration in the waters.

The main objective of the study of the Cúllar-Baza and Padul basins was to obtain palaeoenvironmental information to be applied as boundary conditions in modelling the palaeohydrogeological behaviour of groundwater systems in this region. The Cúllar-Baza lacustrine archive has recorded information about precipitation and palaeotemperature regimes in the stable isotopic compositions of ostracods. The Padul peat bog archive contains a wide range of information in fossil pollen and biomarkers about vegetation and palaeohydrological input. Palaeoclimatic data obtained from these two sites has been used to estimate the palaeoclimatic history at the Los Ratones site.

### 5.1.2 Geochemical Data and Palaeohydrogeological Information

The youngest stage of the secondary minerals paragenesis found in boreholes SR-3 and SR-5 at Los Ratones comprises low abundances of calcite and ankeritic (i.e. Ca-Mg/Fe) carbonate. The carbonate minerals show some zoned growth which is evident under CL examination. This is the only direct evidence of fluctuating conditions during precipitation of these late stage minerals sufficient to cause variations in Fe and Mn contents. There is also minor U mineralisation, showing that conditions have at some time facilitated remobilisation of U from primary mineralisation. A U-Th age on one sample indicates an age in the order of 200,000 years, supporting the relevance of these processes to the PA timescale.

Palaeoenvironmental evidence from geochemical proxies at the Cúllar-Baza and Padul research sites has enabled a clearer link to be established between climate change and hydrological conditions. The range of $^{18}O/^{16}O$ ratios in calcite from ostracods in the lower-to-mid Pleistocene sequence in the Cúllar-Baza Basin is 16‰, indicating a large effect of evaporation during warm episodes as well as of direct terrestrial temperature variation between glacial and interglacial periods. Moreover correlation of $\delta^{18}O$ and $\delta^{13}C$ in these calcites suggests that the basin is endorheic and that its basic hydrological and hydrogeological character changed through the Pleistocene. A similar picture emerges from organic geochemical proxies and $^{13}C/^{12}C$ for the Padul peat sequence which covers an earlier part of the Quaternary than Cúllar-Baza. In the early-to mid-Pleistocene (1 Ma to 400ka), a wet climate prevailed, with deeper surface waters and runoff likely to enhance recharge to groundwater. After that, up to the northern latitudes deglaciation at 180ka, conditions alternated between wetter and drier. In the recent glacial cycles from 170 ka, cold episodes and subsequent deglaciations corresponded with wetter conditions and the Eemian interglacial corresponded with arid conditions. Thus it is certain that recharge to groundwater has varied over the long term and that there were periods in the past (e.g. around 10 ka ago) with lower recharge that at present.

The pattern of alternating 'warm-arid' and 'cold-humid' episodes in the Iberian Peninsula is quite different to the climate-hydrology relations in northern Europe, where relatively arid conditions were associated with the prolonged periods of permafrost during glaciations. The information from Cúllar-Baza and Padul provides a strong qualitative confirmation of the water balance modelling approach using the VISUAL-BALAN code to estimate time-dependent variability of recharge as a boundary condition for the groundwater flow and reactive transport model of the Ratones groundwater system.

Modelling of the Ratones fracture-dominated groundwater system shows that the rate of secondary calcite precipitation, the balance between dissolution and precipitation for both calcite and silica, and the penetration of oxidising conditions versus precipitation of pyrite are all sensitive to recharge rate. Modelling also suggests that redox conditions are likely to be buffered by the pyrite-goethite (Fe-oxide) couple at the depths of investigation. Siderite dissolves under those conditions and the model suggests that siderite budget may influence switches in redox conditions corresponding to recharge rates and thus also to climate changes. At greater depths, pyrite dominates redox control in the model and thus Eh is likely to be more negative.

These modelled variations in the systems can be compared with the evidence from site investigations. The dominant secondary minerals at Ratones are clays, mostly smectite, and carbonates are found mainly in core samples from intermediate and deep boreholes (SR-4 and SR-5) in the southern, down-gradient, part of the system. Present-day groundwater compositions are generally consistent with the secondary mineral distribution, so there is not recognisable evidence of distinctive palaeohydrogeology in the mineral assemblage. Indeed the up-gradient part of the system is found to be dominated by dissolution reactions by which pyrite and ankerite carbonate are being progressively removed from the fracture assemblage, and only in the down-gradient part is there evidence that Fe-rich carbonate may be actively precipitated.

Evidence about redox conditions is also mainly limited to the present regime, there being only weak indications of compositional zoning in carbonates and sparse pyrite in borehole SR-5 down to 500m depth. The relationship between uranium mineralisation in fractures and dissolved U in groundwaters is similarly controlled by dissolution and hydrodynamic mixing, and the chronology and palaeohydrogeological conditions that have controlled secondary U mineralisation are not clear.

Groundwaters with ages from very recent to more than ten thousand years are present in the system, but palaeohydrogeological information from secondary minerals and the hydrochemistry itself do not contain clear signals that link with the palaeoclimate and hydrological record from Cúllar-Baza and Padul. However a general assessment of all of these various types of information indicates that EFEPs for PA scenarios at this type of site should include depth-dependent and time-dependent variations of flow, hydrochemistry and possibly also redox.

## 5.2 ÄSPÖ AND LAXEMAR, SWEDEN

### 5.2.1 Background

Äspö and Laxemar are situated on the Baltic coast of southeast Sweden. The two areas are just a few kilometres apart, Äspö being a small low-lying coastal island and Laxemar being situated inland and to the west of Äspö. The geology of the area comprises intrusive granitoids ranging from quartz monzodiorites to granite. SKB has an underground rock laboratory (Hard Rock Laboratory, HRL) at about 500 m depth on Äspö where it is carrying out a programme of investigations to develop and test methodologies for its programme of research into the storage of spent nuclear fuel. Around 20 core boreholes have been drilled from the surface down to various depths (200 to 1700 m) within the area. In the previous EQUIP palaeohydrogeological project, samples collected mainly from Äspö drill cores were studied. PADAMOT investigations have focussed on mineralization from borehole KLX01, which was drilled down to 1070 m depth at Laxemar.

The postglacial evolution of the area has been strongly influenced by a complex interplay between global sea-level changes, fresh water run-off from the surrounding terrain, and glacio-isostatic fluctuations in the land surface. Consequently, the sites have experienced several different episodes during which either fresh or brackish water environments developed after the last glaciation, and which have had a large influence on the present groundwater chemistry.

The following evolution of groundwater through the Quaternary glaciations and the Holocene deglaciation starting at 13,000 to 14,000 years BP has been inferred from interpretation of their chemical and isotopic compositions:

- Deep recharge by glacial melt water due to high hydraulic heads in the ice sheet and groundwater mixing at considerable depth with a saline water of brine-type.
- Brackish/saline water has been introduced by density turn-over at various stages of the pre-Baltic (Yoldia and Litorina) and Baltic Sea. The present-day brackish water conditions of the Baltic Sea were established around 2,000 years BP and have remained constant to the present day.
- Since Äspö rose above sea-level at around 4,000 years BP, meteoric water has been recharged and mixed with the earlier mixed groundwaters.

### 5.2.2 Geochemical Data and Palaeohydrogeological Information

Previous stable isotope analyses of secondary calcites at Äspö, including those reported in the EQUIP project, found low temperature calcites precipitated from brackish and marine waters down to depths of around 500 m. Small amounts of calcite that had possibly precipitated from meteoric groundwaters containing components of somewhat colder climate waters (i.e. portions of glacial meltwater) were detected at greater depths, possibly down to 1000 m. New studies in PADAMOT suggest that meteoric water penetration might have been even deeper at Laxemar than at Äspö, whilst brackish-marine water penetration was less deep. This is consistent with observations of the present-day hydrochemistry and also with palaeohydrogeological inferences based on the hydraulic effects of land uplift and shoreline displacement. However it is notable that, unlike data from Äspö, stable isotopes have not indicated the presence of calcite with a significant cold climate water signal in deep samples from Laxemar. It is now thought possible that the EQUIP data for Äspö calcites might have overestimated the cold climate water component, due to poor drillcore quality and the lesser use of morphology to select samples that are representative of late stage calcites. The present study has further emphasised the importance of integrating stable isotopes, Sr isotopes, morphology and compositions in the interpretation of whether calcites have late-stage (i.e. Quaternary) origins. Mistaken identification of hydrothermal calcites as late stage calcites puts erroneous weight on the evidence for cold climate waters in the past.

The latest stage of the secondary minerals paragenesis in Laxemar borehole KLX01 comprises small amounts of euhedral calcite, ± pyrite, small quantities of clays (chlorite, etc) on the outermost surface of potentially-conductive fractures, which are mostly partially filled with much earlier mineralisation hydrothermal, and Fe-oxide in near surface (<50-100 m) samples. Caution is, however, required when interpreting this assemblage – it is probably a discontinuous record of groundwater conditions that over-represents the 'precipitating' periods of hydrochemistry, as opposed to 'dissolving' periods. Local redistribution of secondary minerals by dissolution-reprecipitation, probably facilitated during periods of microbial viability and activity, is also thought to be a factor behind what has been observed.

It is suggested that variations in microbial activity over time and with depth is a significant factor in hydrogeochemical conditions. This is likely to be related to the variation over time and depth of traces of dissolved organic carbon in the system. Propagation of microbial activity and trace organics to intermediate depth at some times in the past is confirmed by low $\delta^{13}C$ values in secondary calcite and by the variability of trace elements Mn and La with depth. The significance for past geochemical conditions of variable CL luminescence among growth zones in secondary calcite, which corresponds primarily to variations in Mn content more than in Fe content, needs to be examined in the context of the modelling carried out in WP4. Overall, the mineralogical and isotopic data suggest that EFEPs should include variability in these complex controls on groundwater compositions possibly including redox, over time and probably down to repository depth though this will depend on the overall groundwater flow regime.

Interpretation of calcite morphologies at Äspö/Laxemar is presently based on an assumption that these variations have the same correlation with salinity as has been established at Sellafield, and also on an assumption that the age of the secondary calcite is within the timescale over which fluctuating palaeohydrogeological conditions would be relevant. Variations of late-stage calcite morphology are greater over the upper 260 m of the Laxemar borehole than was recorded from Äspö samples, suggesting that salinity down to this depth at Laxemar was variable in the past. There are very few samples from 260 to 800 m at Laxemar and those few samples tend to correspond to fresh water conditions, but comparisons are not justified. Movement of the position of the fresh-saline interface at Laxemar should therefore be considered in the screening of EFEPs for scenarios in a safety case. Moreover the localisation of changing calcite morphologies within fracture zones suggests that transmissivity of these zones has a stability and longevity, though the timescale is not quantified. Thus continual fracture re-activation is supported and an EFEP of time-dependence for fracture transmissivity might be discounted in this case.

Of particular interest at borehole KLX01 is the existence of calcite with fresh water morphology in a steeply dipping fracture zone at 840-950 m, at which depth present groundwater is saline. This is clear evidence of past deep penetration of fresh water which contributes to an EFEP describing time-dependent changes of groundwater flows in response to uplift and shifting shoreline. It is not a surprising observation in the light of fresh water existing presently at comparable depth in the nearby borehole KLX02. The paragenesis of secondary minerals analysed in samples from 910 m, comprising successive episodes of calcite precipitation from saline groundwater, calcite dissolution and minor clay formation, and further calcite precipitation in fresh water, also indicates that hydrodynamic change even at depth has proceeded as a smooth evolution. Stable isotopic compositions of fresh water calcites from 800-950 m depth in KLX01 indicate that they did not precipitate from a fresh water of dominantly cold climate origin, although this does not preclude minor components of such water.

In conclusion, palaeohydrogeology offers much information to support EFEP definitions for this site. It is evident that groundwater salinity has changed over time at the depths of particular interest for PA, especially where steeply-dipping fracture zones provide transmissive connections from surface to depth. Whether deep fresh water incursions here involved dominant portions of cold climate waters at some times in the past is not clear. Stable isotopic compositions of secondary calcites do not so far record such an episode, although present-day groundwaters are known to retain a minor component of cold climate water. The range of fluctuations of other hydrochemical conditions, especially redox, is also unclear: compositional zoning is not apparent in calcite, though the low quantities prevent definitive analysis, and redox-related evidence of microbial activity, biogenic dissolved inorganic carbon, Mn and La suggests some fluctuations down to about 600 m depth. The persistence of pyrite in the late stage assemblage suggests that any fluctuations have been limited within a range of generally reducing conditions though an EFEP should consider the possible implications.

## 5.3 SELLAFIELD, DOUNREAY AND CLOUD HILL, UK

### 5.3.1 Background

The Sellafield study site is located on the Cumbrian coast of northwest England. The area was investigated by Nirex between 1989 and 1997 to determine whether it would be suitable to host a deep geological repository for intermediate- and low-level radioactive waste. Sellafield lies on a coastal plain, about 10 km wide, between the Irish Sea to the west and the Lake District hills. The bedrock geology consists of an eastwards-thinning wedge of Permo-Triassic sedimentary strata, which overlap Carboniferous rocks resting on fractured crystalline basement rocks of the Lower Palaeozoic Borrowdale Volcanic Group (low-grade regionally-metamorphosed volcanic rocks). This marks the north-eastern margin of the large Mesozoic East Irish Sea Basin. basement rocks.

Twenty-nine boreholes (mostly cored) were drilled within an area of 8 km by 6.5 km, the deepest reaching 1950 m depth. Detailed petrological studies of the fractures and associated mineralization were carried out for Nirex and also as part of the EQUIP palaeohydrogeological investigations. These studies demonstrated a close relationship between the distribution of late-stage calcite fracture mineralisation and present-day groundwater flow. The morphology and microchemical characteristics of the calcite vary systematically with groundwater salinity, and could be used to differentiate calcite precipitated in freshwater and saline water. Morphological and fluid inclusion evidence suggested that the bulk of the late stage calcite formed from groundwaters similar to those at the present day, however detailed petrographical analysis of growth zones in calcite from the freshwater-saline water mixing zone indicates changes of morphology during calcite growth. It was concluded that the morphology of calcite as it has grown is an indicator of the evolution of groundwater salinity especially at the mixing zone between fresh and saline water masses and thus is an indicator of the long-term hydrodynamic stability of the groundwater system.

The conceptual model of the groundwater system of the Sellafield region comprises three discrete regimes: (i) Fresh to brackish groundwater in the coastal plain in which flow is topographically driven and recharged directly. (ii) Halite-derived brines from the Irish Sea Basin, occurring at depth in the western part of the site beneath the present coastline. (iii) Groundwater in the hills to the east of the site and in the basement within the site in which flow is topographically driven with the additional effect of density variations in deep saline groundwaters. The movement of interfaces between these bodies of groundwater at Sellafield is symptomatic of the hydrodynamic evolution and stability of the groundwater system and also might have affected its geochemical stability.

PADAMOT studies sought to test whether the relationships between these characteristics of late-stage calcite and groundwater chemistry that are observed at Sellafield are also useful for palaeohydrogeology at other sites. The specific objectives of the studies were to:

- Evaluate further the relationships between late-stage calcite mineralisation and the evolution of the modern groundwater system at Sellafield;
- Compare relationships between late calcite and groundwater compositions at Sellafield with those at other UK sites, to evaluate their application as a more generic palaeohydrogeological tool.
- Investigate whether calcite mineralisation associated with the development of present-day deep groundwater system records the impact of past climatic changes during the Quaternary.

Secondary calcite mineralisation was sampled from a deep borehole that had been drilled at Dounreay in northern Scotland and from Carboniferous Limestone at Cloud Hill in the English Midlands.

Dounreay is located on the Caithness coast of northeast Scotland. The site was investigated by Nirex between 1989 and 1994 to determine whether the site would be suitable to host a deep geological repository for intermediate- and low-level radioactive waste. It lies on a relatively narrow coastal plain of Devonian sedimentary strata which extends 2 to 3 km to the south and merges with a series of low hills whish are outcrops of the crystalline basement which lies under the Devonian sedimentary rocks at the Dounreay site. The basement rocks comprise a complex series of Precambrian metasedimentary rocks (dominated by migmatitic psammites) generally correlated with the Moine Supergroup. These are cut by two major igneous intrusions, the Strath Halladale Granite and Reay Diorite. The complete sequence is cut by a network of predominantly extensional NE-SW-trending and NW-SE-trending normal faults forming a grid on a scale of 500 m to 700 m.

Groundwater flow is predominantly fracture-controlled in both the crystalline basement rocks and in the overlying Devonian sedimentary cover rocks. The Devonian strata thin rapidly southwards and the crystalline basement rocks form low outcrops rising to 200 to 300 m OD. The principal groundwater flow direction is from south to north, with recharge in the low hills to the south of the site. The groundwater is considered to flow northward and downward, along bedding-related and fault-related fractures, to a zone of discharge and upward flow in the Dounreay coastal plain and possibly offshore.

Two boreholes were drilled and cored at Dounreay, the deepest reaching a depth of 1327 m, penetrating 375 m of Devonian sedimentary rocks and 950 m of crystalline (mainly psammitic) metamorphic and igneous rocks.

Cloud Hill is one of a number of Carboniferous Limestone inliers in northwest Leicestershire, in the East Midlands of England. Samples were collected from the base of a large quarry in fractured dolostone and limestone that is being worked for aggregate. The sequence is highly fractured and extensively dolomitised and is unconformably overlain by red-bed mudstones and siltstones of the Triassic Mercia Mudstone Group. The Carboniferous strata have been affected by karstification, probably of Permo-Triassic age, beneath the unconformity.

The highest point of the site, on the eastern face of Cloud Hill Quarry, has an elevation of 111 m, and the bottom of the quarry is at about -10 m elevation. Groundwater in the Carboniferous Limestone is most probably recharged locally and discharges from open fractures in the base of the southern end of quarry in which late-stage calcite was found. Samples of this late-stage calcite mineralization, plus groundwater from the same fractures, were collected and analysed.

### 5.3.2 Geochemical Data and Palaeohydrogeological Information

*Sellafield*

Late-stage calcite occurs most commonly in fractures in both the Permo-Triassic sedimentary rocks and the Borrowdale Volcanic Basement rocks in the eastern part of the Sellafield area. Its occurrence is limited in the western part of the area where the rocks dip underneath the coast. Morphologies of late stage calcites that are revealed by luminescence zoning in CL studies suggests, in the predominant number of late stage calcites studied, that the fresh-to-brackish water transition has been shallower in the past, i.e. the salinity has decreased over time. Observed morphologies in a few late stage calcites suggest that the opposite has been the case, i.e. the fresh-to-brackish groundwater transition has been slightly deeper in the past and that the salinity in this depth interval has increased over time. These apparently conflicting pieces of evidence may be explained as the result of fluctuating location of the saline transition zone and different calcites having grown over different time intervals. The overall palaeohydrogeological significance seems to be that hydrodynamic conditions have fluctuated either side of present-day hydraulic gradients, at least in the shallow part of the system above the saline groundwater body.

Geochemical variation and growth zoning (as revealed by CL) in calcite indicate that geochemical conditions fluctuated over time and were more localised in up-gradient locations in the eastern part of the area and above the saline transition zone. Geochemical changes deep in the saline groundwaters are represented by fewer CL-distinctive zones that are replicated in samples from several boreholes, i.e. they represent more general geochemical changes. Fe and Mn variations do not have clear relationships with the degree of CL activity, though overall Fe and Mn are much higher in calcites in saline conditions than those above the saline transition zone. There is also a clear correlation in freshwater calcite between low CL activity (i.e. non-luminescence due to low Mn and Fe) and low concentration of the REE cerium ('Ce anomaly'). In summary, these data from CL and trace element (Fe, Mn, Ce) analyses indicate that redox conditions have undergone changes that have probably been fairly substantial in the shallower, fresh water parts of the groundwater system. There have also been changes in the deeper system, as indicated by CL, Fe and Mn variations, but these changes have probably had smaller ranges of variation. The magnitude of redox variation cannot be quantified uniquely from Fe and Mn data, as explained by the modelling carried out in WP4 of PADAMOT, but these data plus consideration of Ce data suggest that fluctuations of redox in the deep saline groundwaters have been within a range that has remained generally 'reducing'.

Some fluid inclusions have higher salinities that present co-existing groundwaters, but inferences that these are hosted in very old growth zones of late stage calcite casts doubt on the palaeohydrogeological significance for the timescale of interest.

Successful microanalyses of the stable isotopic compositions of discrete growth zones, especially those for $\delta^{18}O$ using the ion microprobe, provide perhaps the most compelling palaeohydrogeological information. There is some correlation between CL activity and $\delta^{18}O$, the brighter growth zones, which tend to be older, having relatively depleted $^{18}O$. However doubt remains about whether these growth zones represent a relevant timescale. The depleted $^{18}O$ calcite zones are identified at about 200m depth (ion microprobe data) and at 400-900 m depth (He-LACE data with poorer spatial resolution and non-specific correlation with zones). These isotopic compositions suggest that the zones grew from waters that had large proportions of glacial melt water. It is noteworthy that the spread of $\delta^{18}O$ compositions at 900 m depth goes to heavier $^{18}O$ values consistent with present water composition, as do ion microprobe analyses of calcite from 1500 m depth. These suggest that glacial meltwater did not penetrate substantially below 1000 m. Conversely, the data indicate that water below 1000 m may have been mostly similar to present-day groundwaters over the period of calcite growth.

Variation in the $\delta^{18}O$ values for calcite growth zones above the saline transition zone indicates clearly that there have been large palaeohydrogeological variations in the present fresh water zone.

In conclusion, these additional geochemical analyses for Sellafield samples consolidate the interpretations that were possible from analyses in the EQUIP project. However they have also highlighted some of the uncertainties and ambiguities in the timescale represented and the palaeohydrogeological information. The information is essentially qualitative, showing that the groundwater system has changed in the past and that the sensitivity to external changes generally diminishes with increasing depth. The evidence relates specifically to the impacts of external changes on 'turnover' of the groundwater volume, groundwater salinity and contents of redox-sensitive trace elements (Fe, Mn, Ce). However it is also evident that water with cold climate origin (e.g. glacial melt water) has penetrated to around 1000 m in substantial quantities in the past. There is also uncertainty about the ages and origins of waters that have reached greater depths in the past and that appear to have been isotopically similar to present water at these depths. The exact significance in terms of redox changes of evident temporal and spatial variations of Fe, Mn and Ce in calcite growth zones and thus in co-existing palaeogroundwaters has various uncertainties (as explained for Fe and Mn in the WP4 report). It is most likely that the observed changes of Fe and Mn contents and in Fe:Mn ratios reflect redox changes that have been induced by hydrodynamic and hydrochemical changes originating in recharge. The magnitude of redox change is attenuated with increasing depths. The geochemical indications of redox also have to be interpreted in the context of other redox indications and agents, notably mineralogy, in this case the localised occurrence of pyrite, and microbial intervention.

*Dounreay*

Late stage calcite in much scarcer in fractures in the sedimentary and basement rock formations at Dounreay than in rocks at Sellafield. Consequently its morphology tends to be dominated by older generations of calcite on which it has precipitated as a thin veneer. In such cases, there is much less consistency in the relationship between apparent morphology and salinity and thus less confidence in a palaeohydrogeological interpretation based only on morphology. The interpretation has further ambiguity due to the lack of correlation between the depth of morphological change inferred from mixed and complex data and the depth of the existing fresh to brackish/saline water transition. The former seems to be at around 150m depth and the latter at below 800 m depth. Whether this saline transition zone in groundwater has been at shallower depth in the past is a matter of conjecture and cannot be assessed further by fluid inclusions of which there are none that are measurable with useful certainty in the late stage calcite.

CL activity and trace element (Fe, Mn, Ce) contents are also less helpful as palaeohydrogeological indicators for Dounreay than for Sellafield. Shallow late stage calcite is mostly luminescent under CL and has less trace element variation (and no Ce anomaly) than late stage calcites from Sellafield. There are greater variations of luminescence and trace elements in deeper (>1000 m) calcites from Dounreay but the significance is not interpretable. Moreover the reliability and significance of low salinity fluid inclusions, apparently correlating with low luminescence, are also not interpretable with certainty. The implication is that fresh water penetrated below the present saline transition at some time in the past and perhaps in a localised flow path, but the evidence is too uncertain for this to constitute useful palaeohydrogeological information.

As is observed in Sellafield samples, $\delta^{18}O$ data for Dounreay calcites indicate that glacial melt water penetrated to at least 450 m depth but less substantially at below 1000 m depth. $\delta^{18}O$ of calcite at around 1200 m appears to link it with very old basinal dewatering rather than with groundwaters over a timescale of interest in the present context.

*Cloud Hill, Derbyshire*

Observations of calcites that are inferred to be 'late stage' demonstrate further the difficulty and uncertainty in making useful palaeohydrogeological interpretations from morphology when the relevant calcite is very sparse and precipitated as a veneer on pre-existing secondary mineralisation. In this case, the pre-existing secondary calcites, and also dolomite generations, are probably related to Palaeozoic basin burial and evolution so are of no relevance for present purposes.

Analyses of redox-sensitive trace elements Fe and Mn, in the late-stage calcite show these to be present at low concentrations and thus probably typical of calcites precipitated in near-surface oxidising groundwaters. Geochemical modelling in WP4 has confirmed that this is a valid, but not unique, interpretation. These low Fe and low Mn, mostly low luminescence (except for relatively minor zones that have higher Mn and are more luminescent) calcites might be considered as analogues for secondary calcites that are definitely representative of shallow environments dominated by oxidising supergene alteration. However the absence of a Ce anomaly indicates that interpretation of the presence of a Ce anomaly, as in the non-luminescent growth zones in shallow calcite from Sellafield, is not simply a matter of oxidising versus reducing palaeogroundwater. Geochemical conditions in the source regions for groundwaters may have as important a role in determining their compositions as the geochemical environment where calcite has been precipitated.

The rather wide range of $\delta^{18}O$ values obtained by ion microprobe and He-LACE analyses of the late stage calcite, both significantly heavier and lighter than equilibrium with present-day groundwaters, is also an indication of possible uncertainties in the palaeohydrogeological interpretation of such data. Three possible explanations can be proposed: actual variations in palaeohydrogeology in the timescale of interest, 'contamination' of analyses by older calcite, or non-equilibrium isotopic fractionations.

## 5.4 MELECHOV MASSIF, CZECH REPUBLIC

### 5.4.1 Background

The Melechov Massif is a Variscan granite body located about 80 km to the SE from Prague and is the northernmost promontory of the Moldanubian pluton in the Bohemian Massif. The area is being used for testing methodologies for the development of a deep geological repository in crystalline rock. The objective of PADAMOT studies at Melechov has been to clarify and update ideas about the shallow origin and circulation of groundwater in the fractured granite and to provide data for hydrogeological modelling.

The region has a complex system of fractures and fracture porosity, related to its long and complex tectonic history. In addition, Tertiary uplift and erosion have significantly modified the land surface and impacted on drainage patterns. Furthermore, weathering and superficial deposits affect the permeability of the fissured zones. These features seem to be the controlling factors on groundwater circulation and residence times. A general investigation objective is to find out if there are deep groundwater circulation systems in tectonic zones and to compare groundwater residence times in fissures with residence times in granites elsewhere in the Bohemian Massif.

Petrological, mineralogical and hydrogeological information was obtained from borehole PDM-1 which was drilled to 100 m depth at the southern foot of Melechov Hill in 2002. A hydrogeological field survey was also undertaken to provide input data for hydraulic modelling of the groundwater flow system. Sixty groundwater samples were collected and analysed in the chemical laboratory of the Czech Geological Service.

Melechov has a particular set of potentially-important EFEPs that define present-day and long-term groundwater movements and siting of a potential repository in this type of rock formation and location. Palaeohydrogeology since the Tertiary period, is thought to have been dominated by weathering, hydraulic gradient increase and potential fracture reactivation that were associated with general uplift of the massif. Thus EFEPs need to describe depth-dependent transmissivity in fracture zones and faults, and lateral connections within the fracture network from the topographic high in the centre to potential discharge areas on the periphery, and whether these characteristics have changed over time.

### 5.4.2 Geochemical Data and Palaeohydrogeological Information

Groundwater ages and other hydrochemical information are the primary source of evidence to define those EFEPs. Isotopic data on groundwater from the borehole at Melechov show that, at this shallow depth range, groundwater is entirely recent recharge and geochemically immature, though some evolution to Ca-Na-$HCO_3$ composition has occurred. Predominance of a pre-existing fracture mineral assemblage of probable hydrothermal origin that comprises Fe- and Mn- oxides as well as chlorite and pyrite (increasing downwards) indicates that redox-controlling reactions may already be occurring but are not yet buffering redox conditions. In other words, the weathering process between infiltration water and existing fracture minerals and wall rock is likely to advance over time in this hydrodynamically shallow zone.

Information from Melechov is limited because the borehole is only 100m deep, but sparse hydrochemical and isotopic data from other locations in the southern Bohemian Massif (i.e. not in the areas of the northern massif where thermal springs represent connected and transmissive fractures that penetrate to anomalous depths) indicate that the distribution of groundwater ages with depth may be rather heterogeneous. Thus an EFEP describing depth dependence of groundwater movement would need to be left open in the present state of knowledge.

# 6 Evaluating Palaeohydrogeological Information with Evidential Support Logic

## 6.1 INTRODUCTION AND OBJECTIVES

The question arises as to how evidence drawn from palaeohydrogeological studies, using the methods and data developed in PADAMOT, can most effectively be used in support of a safety case for the deep geological storage of radioactive waste. In 2004, Nirex invited Quintessa to undertake a demonstration of the potential application of Evidential Support Logic (ESL), as a contribution to PADAMOT, with the aim of providing a structured logical analysis of the use of palaeohydrogeological evidence in support of site evaluation and safety case development. Specifically, ESL was to be used to determine the degree of support for the statement that "environmental change at the surface has little impact at repository depth".

ESL is a methodology for assembling evidence from diverse sources in a coherent decision support model (Bowden, 2004; Metcalfe et al., 2002; Seo et al., 2004). It formalises and makes transparent the subjective processes of expert judgment that are inherent in drawing general conclusions from detailed supporting evidence, taking account of the sources and implications of uncertainty. However, ESL is intended to be used with all relevant evidence being brought to bear in a common decision support model. Evidence might include 'hard' quantitative data and the results of quantitative modelling alongside analogue reasoning and expert judgment of 'soft' information. Moreover, whilst there may be a large volume of information relating to a decision, much of it may be only of partial relevance, incomplete or even sometimes conflicting.

'Bias' in decision making can arise when one particular source of evidence is relied upon to an excessive amount, regardless of the inherent uncertainty or the weight of contradictory information. Therefore, focusing attention on the role of one specific category of evidence, such as the palaeohydrogeological methods used in PADAMOT, is an incomplete and potentially biased application of ESL.

Nevertheless, the ESL approach may be useful for evaluating palaeohydrogeological information which has involved 'implicit interpretation' for which the confidence cannot be easily assessed (Bowden, 2003). In order to make effective use of such palaeohydrogeological information in PA, it is necessary to make judgments on both the quality of the data and the quality of the interpretation and modelling process.

An expert group of UK partners in PADAMOT made judgments of the availability, significance and reliability of palaeohydrogeological evidence for past groundwater conditions in the Sellafield area and the corresponding external features, events and processes (EFEPs). These judgments also incorporated knowledge and understanding of other types of evidence (including modelling, regional geomorphological evidence, etc).

The general principles behind the use of ESL are described in detail in Appendix B, as are the detailed procedure and outcomes of applying ESL to palaeohydrogeological evidence from Sellafield.

## 6.2 SUMMARY CONCLUSIONS FROM USING ESL

A brief summary of the main points arising from the trial application of ESL is given here. The full discussion of outcomes and recommendations is in Appendix B.

The ESL model of palaeohydrogeological evidence applied in this study inevitably invoked consideration of a wider range of types and sources of evidence than from the PADAMOT palaeohydrogeological project and, being focused on the implications for scenario selection for PA, it was recognised that some areas of the model cannot be addressed by geochemical and mineralogical data alone. The complex decisions required by ESL rely on broad-ranging consideration and manipulation of a range of types and sources of evidence with relevant uncertainties. Therefore the full potential evidence base needs to be recognised and an appropriate interpretative and ESL model structure has to be developed.

The broad conclusion of this exercise is that the isolated use of palaeohydrogeological data and interpretations of the types involved in PADAMOT do not, in their current state of data density and interpretative uncertainty, provide a strong basis for making unequivocal judgments on PA scenario-related decisions. This conclusion also appears to be the view of many people involved directly in PA work, as illustrated by the reviews of PA exercises in Section 1 of this report.

Despite the above difficulties and caveats in using ESL in the PADAMOT context, the process that was followed in developing logical models to use palaeohydrogeological evidence in support of scenario development illustrates how this type of information could be framed to be usable by PA teams. The formalised approach engenders critical thinking about the way in which such evidence is assessed and interpreted, testing the credibility of judgments and interpretations of relevant data for their use in constraining scenarios in PA.

Scenario development for PA requires that all sources of evidence and judgement relating to the analysis of both past and potential future changes are deployed. ESL can help to ensure that assessment modellers, site investigators and geosphere/biosphere researchers, rather than being ‘compartmentalised’, work together within a single team with the common aim of challenging safety arguments and identifying, understanding and resolving uncertainties. Otherwise there are likely to be unresolved inconsistencies between interpreted palaeohydrogeological information and the scenarios adopted for performance assessment.

# 7 Conclusions and Recommendations

The review of existing PA exercises in Chapter 2 shows that palaeohydrogeological information has been fairly widely used to support, directly and indirectly, the conceptual model for site evolution in base/central scenarios or in variant scenarios. In many cases, theory-based concepts for scenario evolution have been supported qualitatively by palaeohydrogeology. The aim of PADAMOT has been to strengthen the ways that evidence-based palaeohydrogeology is used to test and quantify the evolution scenarios being used in PA. PADAMOT has focused on palaeohydrogeological evidence from mineralogical and geochemical analyses and interpretations.

Chapter 3 has recommended that the most effective way to channel information from palaeohydrogeology into PA is by translating the evidence explicitly into 'external' FEPs (EFEPs; Table 3.1). These EFEPs are important in scenario development for PA because they provide information about boundary conditions of the groundwater model and about the chemical properties of the geosphere, redox, pH and salinity, to which near-field conditions and radionuclide mobility may be most sensitive. To transfer this information effectively, it is necessary to appreciate how PA experts use EFEPs to describe scenarios and where in that process are the qualitative and quantitative interpretative models that would be constrained with palaeohydrogeological information.

The proposed method of using palaeohydrogeological information requires that (i) the construction of scenarios by the PA group is done by the process shown from the top downwards in Figure 3-1 to assess the possibilities for climate-driven disturbance of the system, and (ii) the interpretation of palaeohydrogeological information by the site characterisation group is more quantitative and explicit in evaluating its significance for EFEPs and the associated uncertainties. The second process here is shown in Figure 3-1 from the bottom upwards and involves using quantitative palaeohydrogeological information to constrain the interpretative models and the estimates of EFEPs.

More details of this process for using palaeohydrogeological information are shown in Figure 3-2. Section 3.2 explains how geochemical and mineral measurements from site characterisation should be put through a systematic interpretation (quantitative, qualitative and expert judgement) to obtain data that are comparable with outputs from the scenario models. A supplementary approach is also shown in Figure 3-2, whereby site characterisation data are used specifically to consider whether there is palaeohydrogeological evidence that climate impacts in the past have been attenuated with increasing depth. If that could be shown, it would build confidence in general principle for geological repositories that deep emplacement in the geosphere will mitigate impacts of future changes at the surface.

Chapter 4 discusses in generic detail the geochemical and mineralogical data sources for palaeohydrogeology and the interpretations that are necessary for screening EFEPs and scenarios. The interpretative approach usually used is a qualitative judgement of significance and, if justified, a semi-quantitative estimate of magnitude of the process. Another approach is discussed and illustrated in Chapter 6. It employs a structured examination of evidence from palaeohydrogeology for specific EFEPs or impacts on the groundwater system (Evidential Support Logic, or 'ESL'). Further discussions below of the significance of palaeohydrogeological information use the first approach; the ESL approach would be most practicable in specific cases where contentious scenarios can be screened against large and diverse site characterisation data and against diverse export interpretations.

The rest of this chapter discusses how well the outputs from WP2, the salient aspects of which are summarised in Chapter 5, contribute to the process recommended in Chapter 3. The discussion also involves the interpretative principles summarised in Chapter 4 and considers the modelling carried out in WP4 to support interpretation. Two areas of focus suggested in Chapter 5 are evidence for (i) discontinuous changes in the groundwater system over a timescale comparable with the PA timescale, and (ii) attenuation of long-term changes in the surface environment with increasing depth.

*Los Ratones*

It is considered that, apart from the anthropogenic changes due to the mine itself, the greatest possibility of discontinuous change in the groundwater system would be fluctuations of the water table and hydraulic gradient synchronously with arid-pluvial cycles of climate. Site investigations have concluded that mineralogy is not a substantial source of evidence for hydrodynamic changes and provides only scant evidence for geochemical changes. Most of the groundwater system that has been investigated so far comprises a slowly weathering geochemical environment, dissolving calcite and not precipitating it. Therefore calcite, which is the main focus of secondary mineral studies in PADAMOT, is not a viable source of palaeohydrogeological information here. The extent to which groundwater conditions have fluctuated over time is not evident from this or other types of geochemical data. Data from chemical and isotopic analyses of groundwaters, carried out outside PADAMOT, are also not explicitly diagnostic of palaeohydrogeology although they assist in identifying the structural controls on flowpaths and hydrochemical mixing in pre- and post-mining groundwater regimes at Ratones.

Geochemical proxies at the Cúllar-Baza and Padul sites are a successful tool in the context of Spanish sites for diagnosing evidence of regional hydrological impacts of past climates. Stable O and C isotopic ratios in calcite from ostracods and organic geochemistry proxies identify those impacts very clearly and moreover can be placed in a discrete chronological sequence due to the success of dating techniques and to the completeness of the Cúllar-Baza and Padul sequences. Stable O isotopes also indicate clearly that intense evaporation has occurred at certain periods, which can be inferred to correspond to episodic water table fluctuations and variations of water compositions. This is valuable input to the VISUAL-BALAN model of time-dependent variations of recharge.

Overall, it can be concluded that the mineralogical and geochemical methods promoted by PADAMOT have not been useful in the shallow weathering regime at Los Ratones. Palaeohydrogeological evidence has not yet been able provide significant support to the successful development of integrated theory-based time-dependent modelling of the groundwater system. However the methods might be useful in any future testing below presently-investigated depths at this type of site to investigate how deeply oxidising and dissolving geochemical conditions have penetrated at different times.

*Laxemar/Äspö*

Mineralogical and isotopic properties of secondary calcites are distinct in the brackish-marine and meteoric-?glacial groundwater regimes at intermediate depths and deep locations respectively in the Äspö and Laxemar systems. The resulting information about past distributions of groundwater masses supplements the palaeohydrogeological interpretation of sampled groundwater compositions by qualitatively indicating the sensitivity of these distributions to temporal changes of boundary conditions. This provides valuable input to scenario development, but its qualitative nature limits its value for testing the validity of palaeohydrogeological modelling. Data are primarily limited by the sampling limitations and challenges imposed by sparse secondary minerals. Two cautionary comments on the PADAMOT methodology are that interpretative models for morphology variations are presently generic and rely on calibrations of morphology versus salinity in Sellafield calcites, and that secondary minerals provide a discontinuous record which omits periods of mineral dissolution.

It has been observed that late-stage secondary calcites are localised in certain fracture zones, with different calcite generations distinguished by their morphologies. This is significant for PA in showing the persistence over time of the spatial distribution of water flow paths.

Overall, the PADAMOT methodology for palaeohydrogeology provides some important indications of the breadth of variability that PA scenarios should consider for the Laxemar/Äspö groundwater systems. As in the Sellafield case below, a quantitative output to interpretative models such as those in Figure 3-2 is, however, not possible.

*Sellafield, Dounreay and Cloud Hill*

Additional petrographic analyses of late stage calcite in drillcore samples from past site investigations at Sellafield in northwest England have consolidated the findings from previous work carried out in the EQUIP project. Morphology variations in overgrowths of late stage calcite have suggested that the position of the fresh/brackish-to-saline water transition zone has fluctuated both above and below its present location, but with additional observations the balance of evidence supports the predominance of a slight downward movement, by at most a few tens of metres, of the transition zone over time, i.e. a dominant trend over time of decreasing salinity at any point in this interval. This indicates that a hydrodynamic and hydrochemical response at 300-400 m depth to changes in the surface environment should be considered in FEPs, but also that the distributions of flow directions in the groundwater system has remained fairly stable over the time period represented by the late stage calcites. Data from various instrumental methods for analysing chemical and isotopic compositions of discrete calcite growth zones suggest that the compositions of groundwaters from which they precipitated changed over time. The patterns of variations support the concept that changes in deep saline groundwaters are more attenuated than in fresher up-gradient groundwaters. In these freshwater calcites, contents of the redox-sensitive trace elements Fe, Mn and Ce are correlated which indicates that the fluctuations in compositions are related to changes in palaeoredox conditions. Thus palaeohydrogeological information suggests that FEPs for PA should consider long-term changes of redox, although it is also evident that the scale of change is attenuated in deeper saline groundwaters. The quantitative significance of the observed Fe and Mn variations has been studied in WP4 by geochemical modelling, which shows that absolute and relative changes in Fe and Mn concentrations have non-unique interpretations in terms of redox (Eh) values.

Samples of secondary calcite from the other UK study sites at Dounreay and Cloud Hill pose an analytical and interpretative problem because the amounts of late stage calcite are low. In both cases the calcite morphologies tend to be dominated by that of older secondary calcite on which late stage calcite has precipitated as a veneer. Uncertainty in calcite characterisation means that the significance of the substantial discordance in the depth locations of the transitions of morphology of late stage calcite and of salinity in the present-day groundwater profile at Dounreay is interpreted with much less confidence than for samples from Sellafield. Variations of redox-sensitive trace elements (Fe, Mn, Ce) are less systematic than at Sellafield although there is a general contrast between trace element contents of shallow and deep calcites with more variation at depth. However there is too much uncertainty and lack of reproducibility in these sparse localised data to interpret reliable palaeohydrogeological information. The few stable isotope data from Dounreay calcites tend to repeat the inference from isotope analyses at Sellafield that glacial or cold-climate water volumetrically replaced pre-existing water down to about 450-500 m depth since late stage calcites below this do not have such light $\delta^{18}O$ values.

*Melechov*

Although this type of site, in the centre of a domed massif, has some potentially important time-dependent EFEPs that might influence scenarios, the PADAMOT methodology is not applicable for the shallow depth interval to which Melechov investigations are presently limited. As is the case for the Ratones site, methods that focus on secondary minerals, specifically calcite, are not practicable for the shallow weathering zone but are likely to become valuable in deeper investigations.

An important aspect of the Melechov massif study is that the general directions of flow paths from recharge to discharge, i.e. from the uplands of the domed massif to the incised rivers at its periphery, are fairly obvious, but the depth dependence of flow and travel times to discharge are not known at all. These latter properties would of course be of central importance for the siting and PA of a repository sited in this sort of hydrogeological environment. The PADAMOT methodology combined with conventional hydrochemical and isotopic studies could provide valuable information about the deep parts of the down-flowing limbs of the groundwater system and about the flowpaths that converge towards groundwater discharge areas at lower elevation.

*Overall conclusion and recommendations*

There is a need to incorporate more palaeohydrogeological information into PA in order to improve the credibility of assumptions about stability of deep groundwaters and of estimates of the likely magnitudes of impacts of external changes in scenarios. This study concludes that the most appropriate way to do that is to use palaeohydrogeology to screen and quantify FEPs that are the basis for developing scenarios to be used in PA. Logical approaches to doing this have been illustrated in this study, showing the considerable steps of data acquisition, interpretation and expert judgement that are involved in attempting to quantify information for transfer into FEPs and scenarios. The process of interpretation and expert judgement is usually carried out by means of a narrative assessment of the evidence, supported by geochemical, hydrodynamic and coupled reaction-transport modelling as illustrated in WP4. A more rigourous approach with ESL has been exemplified here but it is likely that the conventional narrative interpretation will continue to be the most practicable approach.

Narrative interpretations have been abstracted into this report from the investigations carried out in WP2 on samples from the various study sites. The principal analytical methods that have been used and evaluated in WP2 are mineralogical, geochemical and isotopic analyses of late-stage secondary calcite. Their applicability depends primarily on the occurrence of late-stage calcite in sufficient abundance for characterisation to be analytically feasible and reasonably reliable. In general, late-stage calcite has grown and been preserved at depths below the weathering zone where groundwater compositions have been continually saturated with respect to calcite. Where these conditions obtain, as at typical repository depths, i.e. below 100-200 m, in the rocks at Sellafield, Äspö/Laxemar and Dounreay, a remarkable amount and diversity of data may be obtainable, though abundance of secondary calcite and the feasibility of sampling are strong constraints on what can be achieved. In other geological and hydrogeological conditions, e.g. in shallow groundwater environments and at earlier stages of site reconnaissance, different sampling and analytical approaches are necessary and are illustrated by the studies at Los Ratones and Melechov.

Even in the most advantageous sampling and analytical conditions, there are substantial interpretative uncertainties associated with the assumptions made in 'expert judgement' and with calibrations of process models. Further basic research to understand the geochemical and mineralogical processes underlying the genesis of secondary calcite, the calcite morphology-salinity relationship, and the distributions of redox-sensitive trace elements in secondary minerals is required to reduce these uncertainties. Nevertheless it is evident from these PADAMOT studies that, by adopting palaeohydrogeological methods that are appropriate to the particular geological and hydrogeological conditions, important qualitative evidence of greater or lesser degrees of stability in past groundwater conditions is already accessible. This 'palaeo' evidence should be taken into account in considering scenarios of future climate changes and their potential impacts on the stability of deep groundwater conditions for repository safety cases.

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# Appendix A: Review of Palaeohydrogeological Information in Safety Cases

## A1 PALAEOHYDROGEOLOGY IN FRACTURED ROCK SAFETY CASES

### A1.1 Kristallin-1, Switzerland (Nagra, 1993)

Alternative scenarios (versus the reference scenario which assumes that conditions continue as at present and that any changes are negligible) for geological and climatic changes were considered in Kristallin-1. Potential geological changes associated with continued Alpine uplift were evaluated and were found to have ranges within uncertainty bounds already applied to reference scenario modelling. Future climate changes were considered by various alternative scenarios including one for periglacial conditions with permafrost, but these mainly affected the biosphere model. Increased geosphere groundwater fluxes and decreased transit times were also considered by varying parameters in the reference scenario. No direct reference to palaeohydrogeology providing limits to the alternative scenarios and their parameter ranges appears in Kristallin-1. The interpretation of regional hydrogeology, including the palaeohydrogeological interpretation of hydrochemical and isotopic data contained in Thury et al. (1994) is cited in support of the stability for reliable operation of the engineered barriers over a long timescale that is provided by the geosphere at 400m depth.

### A1.2 AECL 94, Canada (Davison et al., 1994)

Canadian regulations at the time of the assessment did not require an evaluation of radiological safety beyond 10,000 years, but palaeohydrogeological studies of groundwater ages and mixing and of fracture calcites were carried out. Stable isotope ($^{18}O/^{16}O$, $^{2}H/^{1}H$) and $^{14}C$ data identify brackish waters in fracture zones at several hundred metres depth that correspond to recharge during the last glaciation, and below there are older saline groundwaters of probable pre-glacial origins (Gascoyne and Chan, 1993; Gascoyne et al, 1999, Laaksoharju et al., 2000; Gascoyne, 2004). Salinity changes and other indications of groundwater mixing indicate that advection of water in present-day recharge conditions does not penetrate much below 200m depth, and cold climate waters in the past have not circulated deeper than about 500m corresponding to a sharp diminution of fracture density (Gascoyne, 2004). Secondary minerals in fractures at various Shield locations were studied by isotopic and geochemical methods from which data were interpreted as indicating episodes of dissolution and precipitation with timing from early hydrothermal conditions to recent groundwater circulation (Bottomley, 1987; Bottomley and Veizer, 1992; Bottomley, 1993; Gascoyne et al., 2003).

### A1.3 SITE-94, Sweden (SKI, 1996)

SITE-94 was the regulator’s independent assessment of a hypothetical repository site with characteristics similar to those at Äspö (i.e. Aberg in SR 97). It was recognised that climate scenarios can be constrained by palaeohydrogeological interpretation of the present-day distribution of salinity. A regional-scale groundwater flow system was inferred to be controlling the age, distribution and mixing of deep shield-type brines and saline groundwaters. Oxygenated glacial meltwater was hypothesised to have penetrated to more than 1000m depth beneath the Pleistocene ice sheets, for which there is evidence in relict water with cold-climate isotopic composition (though the possibility of water remaining oxidising to that depth is disputed by SKB, referring to mineralogical and geochemical modelling evidence that dissolved oxygen is attenuated by reaction with ferrous minerals at shallow depths) (Guimera et al., 1999).

SITE-94 states that 'geochemical modelling for prediction of possible future changes at a given site and the consistent description of the variability in geochemical parameters….. must be based on an understanding of how observed geochemical phenomena have developed due to past and present processes'.

Scenario identification in SITE-94 was done in terms of EFEPs (external FEPs). The Reference Case involved no changes of the EFEPs over time. A Central Scenario for 120,000 years into the future was developed incorporating changes over time in the EFEPs that concern climate, i.e. permafrost, glaciation and sea-level changes. Assessing the impact of the Central Scenario was aided by quantitative or qualitative information on how past climate events were interpreted as having affected the geosphere (King-Clayton et al., 1995).

### A1.4 Nirex 97, UK (Nirex, 1997a)

The Nirex 97 assessment of post-closure performance of a repository at Sellafield in northwest England was carried out with a groundwater model that assumed steady state conditions, i.e. it used the present-day hydrogeological setting, boundary conditions and measured parameters. Clearly, over the assessment timescale of up to a million years, this assumption would not be valid and transient modelling or steady state modelling with varying boundary conditions would be required, as Nirex had planned beyond Nirex 97. Palaeohydrogeological information was not explicitly used in Nirex 97 to assess the extent to which the groundwater system at Sellafield had deviated from uniform steady state flow over timeframes in the past that mirror the future timeframes for assessment: $0\text{-}10^4$, $10^4\text{-}10^6$, and $10^6\text{-}10^8$ years. However interpretations of hydrochemical, isotopic and mineralogical data were covered in a supporting report (Nirex, 1997b; Bath et al., 2004) and hydrodynamic models of the evolution of the site were used (Golder Associates, 1995). Both of these aspects of palaeohydrogeological analysis provided input to the developing conceptual model of the site.

Stable isotopic and $^{36}Cl$ data indicated contrasting turnover times in different parts of the groundwater system at Sellafield. Stable isotopes show that cold climate water, presumed to be of Pleistocene recharge age (i.e. between 1.6 million and 10,000 years old) has moved through the onshore basement rocks to the maximum drilled depth of 1700m. $^{36}Cl$ suggests that brine in the coastal and offshore sedimentary and basement formations has been stable for a longer period, in excess of 1.5 million years. At the boundary between this offshore basinal system and the onshore groundwater system, $^{36}Cl$ indicates that saline water movement between sedimentary and basement formations has occurred during the Pleistocene. Information from secondary calcite also indicates long-term stability in the overall system although it also indicates varying degrees of relatively minor fluctuations of salinity and redox conditions, varying over different flow regimes, i.e. shallow or deep basement, inshore or coastal.

Studies of secondary mineralisation in both sedimentary and basement formations established an understanding of past groundwater flow pathways and likely geochemical conditions. Detailed studies of the complete parageneses of secondary mineralisation allowed the most recent 'late-stage' fracture mineral assemblages to be distinguished from older deposits. These late-stage mineralisation episodes (ME) were interpreted to be associated with groundwater circulation during the Tertiary and Quaternary periods. The dominant mineralogical features of these late-stage episodes are Fe/Mn-oxyhydroxide mineralisation (ME8), dissolution of dolomite and anhydrite (associated with ME8 and ME9), and widespread calcite mineralisation (ME9) (Nirex, 1997c; Milodowski et al., 1997). Widespread ME9 calcite is thought to be the latest phase of mineralisation from groundwaters flowing through the fractured rock. ME9 calcite is almost always found in unsealed fractures and fissures and its occurrence was used to identify 'Potential Flowing Features' (PFFs) as information to supplement hydrogeological logs.

Thus palaeohydrogeology provides significant input to the groundwater pathway modelling that would underpin a safety case for Sellafield, although it was not used directly in Nirex 97.

## A1.5 SR97, Sweden (SKB, 1999)

SKB's safety case exercise SR97 was based on three generic sites (Aberg, Beberg and Ceberg) that were parameterised by data sets from three SKB research sites: Äspö, Finnsjön and Gideå respectively. Land uplift is a known trend and is included in the base scenario, whilst climate change and its potential impact on groundwaters are considered variant scenarios. Therefore hydraulic and hydrochemical evolution of the geosphere due to land uplift only is included in the base scenario and evolution due to other time-dependent changes is comprehensively included in the variant climate scenario. The climate scenario particularly hypothesises on the transient groundwater flows associated with glaciation and permafrost.

Palaeohydrogeological interpretation of hydrochemical, isotopic and mineral data from the three generic sites informed the discussions of hydraulic and chemical evolution in the climate scenario of SR97, though this is not explicitly acknowledged and explained. Conceptual models for future evolution of the geosphere at the three sites are constructed to resemble past evolution as inferred from interpretations of present groundwater conditions. Effects of future climate change at the three sites differ considerably in the expected durations of ice cover and submergence beneath the sea. By analogy with interpreted palaeohydrogeology, the hydraulic and chemical conditions also differ considerably. The magnitude, spatial extent and timing of these changes are studied by modelling that is validated through simulation of past changes up to the present and comparison with observations, for example, with the depths of penetration and the degree of mixing/dilution of glacial meltwater and of post-glacial Baltic seawater (Svensson, 1999a, 1999b, Laaksoharju et al, 1998).

Another significant comparison between predictive modelling and palaeohydrogeological information is that between a geochemical model of reductive buffering of oxygenated infiltration by rock minerals and observations of the spatial distribution of secondary mineralisation by iron oxides (Guimera et al., 1999; Gascoyne, 1999). Modelling of the glacial scenario is predicated on the hypothesis that the greatest downwards hydraulic pressure and potential flux of fresh oxygenated melt water will occur while the margin of the ice sheet is passing over the repository location. Modelling of the permafrost scenario is predicated on the hypothesis that groundwater flow will be restricted to greater depths by the reduction of permeability due to freezing at shallow depths with a consequent reduction in recharge, and also on the suggestion that saline groundwater may be generated by freeze-out as a by-product of pore water freezing. So far, palaeohydrogeology has not produced firm evidence to confirm these hypotheses, although field and laboratory studies at the Lupin Mine (northern Canada) have produced various bits of controvertible evidence (Ruskeeniemi et al., 2002, 2004).

The combined effect on groundwater flow and specifically on potential radionuclide transport of geosphere and biosphere conditions in the glacial climate scenario is significant as an increase of dose relative to the base scenario for only one of the three sites – Aberg. In this case, a fall of the relative shoreline during an interglacial transition to a glacial climate exposes previously submerged areas and therefore modifies the biosphere. The site-specific scenario was not supported explicitly by palaeohydrogeological interpretation of groundwater data, though considerable interpretation using a mixing model has been published for that site (Laaksoharju et al., 1998, 1999; Laaksoharju, 1999). The overall conclusion in SR97 is that, for the majority of situations considered, even extreme climate change does not substantially affect the safety of a repository. Palaeohydrogeological interpretation of site data is playing a large role in the development of site descriptive models at SKB's candidate sites at Forsmark and Simpevarp. It is recognised that this approach offers important possibilities both for confirming the parameterisation of the base case model and for constraining the scale of change envisaged by the climate scenario (Smellie et al., 2002; Laaksoharju et al., 2004a, 2004b; SKB, 2004a, 2004b).

### A1.6 TILA-99, Finland (Vieno and Nordman, 1999)

Posiva's safety assessment for four candidate repository sites started out with conceptual descriptions of 'normal evolution' of the natural and repository systems. The normal evolution of TILA-99 is equivalent to the base scenario in SKB's SR97. The normal evolution description is divided into five timeframes; up to 100 years, 100 to $10^4$, $10^4$ to $10^5$ years, $10^5$ to $10^6$ years and beyond a million years. These descriptions of normal evolution and the potential effects on the repository system and on geosphere conditions are constrained by palaeohydrogeological interpretation of hydrochemical, isotopic and mineral data especially the observed distributions of salinity at the four sites (two of which are coastal and two are inland), the groundwater ages interpreted from stable isotopic and $^{14}C$ data, and distribution of oxidised iron-containing fracture-fill minerals (Pitkänen et al, 1996, 1998a, 1998b, 1999). Palaeohydrogeology indicates that post-glacial land rise and eustatic sea level change have had significant impacts on the evolution of groundwater flow over time at the two coastal sites. The groundwater flow model used in the assessment assumes steady state, but then scenarios were explored by qualitative or semi-quantitative 'what if' variants. The hydraulic and hydrochemical conditions and boundaries of these variant models were strongly constrained by palaeohydrogeology for glacial meltwater, fresh-water flow, and saline groundwater scenarios.

Overall, the basis of PA has been conditioned by the understanding of past meteoric waters in the uppermost 150-2000m (or more for inland sites) and of the stable saline groundwaters at depths greater than 750m.

Since TILA-99, there has been increasing interest in the past evolution of the saline-fresh water transition at Olkiluoto in the context of potential upconing of saline groundwater towards an excavated repository.

### A1.7 H-12, Japan (JNC, 1999)

H-12 focused on the perturbation scenarios of seismicity, volcanism, uplift and erosion and did not have a climate change scenario. These scenarios were assessed qualitatively or semi-quantitatively as variants on a base scenario which assumed uniform steady state groundwater conditions. A scenario associated with global climate change to a glacial period would involve eustatic fall of sea level and the replacement of saline water by fresh water at a coastal repository site. JNC does not have a coastal research site at which the palaeohydrogeological evidence to support this scenario could be studied – the Horonobe site is 15 km inland and the now-closed research site at Kamaishi, though near a coast, is 250-550 m above sea level. Palaeohydrogeological studies at two research sites at Tono and Kamaishi have provided information on the evolution of groundwater systems in faulted rock areas that are subject to repeated seismic events. A study of fracture-fill material in the Nojima fault zone, responsible for the 1995 Kobe earthquake, showed that fracture-fill calcite down to 1800m depth has formed from infiltration of meteoric and sea waters within the last 60,000 years (Lin et al., 2003).

### A1.8 AGP-Granite, Spain (Enresa, 1997)

AGP (Almacenamiento Geológico Profundo) performance assessment exercises carried out by Enresa looked at potential safety issues for hypothetical deep repository sites in generalised 'type' sites in granite and clay. The methodology included the development of scenarios and identification of FEPs which defined a reference scenario (base case) and alternative scenarios. The only two alternative scenarios for which potential consequences were assessed involved human intrusion and failure of a shaft seal in AGP-Granite (a deep water well and shaft seal failure were the alternative scenarios for the parallel exercise for a clay site, AGP-Clay; Enresa, 1999). Enresa have compiled and evaluated the evidence for how global climate change will affect hydrological, hydrogeological and biosphere systems and considered the implications for scenarios for sites in the Iberian Peninsula (Recreo and Ruiz, 1997). Palaeohydrogeological information to support scenario development has been obtained by studying travertine and speleothem (Torres et al., 1996). This information has been integrated with palaeoclimatic information from palynology, organic chemistry of 'biomarkers' and stable isotopes ratios.

## A2 PALAEOHYDROGEOLOGY IN OTHER SAFETY CASES

### A2.1 SAFIR-2, Belgium (ONDRAF/NIRAS, 2001a)

The safety assessment and feasibility report for a proposed repository in the Boom Clay implicitly considers palaeohydrogeology through the hydrochemical data and interpretation. Aquifers beneath the Boom Clay have relatively elevated salinity, indicating mixing with relict depositional seawater of Tertiary age.

The influence of climate change on the transport of radionuclides from a repository at Mol/Dessel in the Boom Clay over the next 125,000 years was studied in the EVEREST project (Cadelli et al., 1996). More recently, other simulations have been conducted as part of a palaeohydrogeological study of the Mol/Dessel site over the last 100,000 years (the PHYMOL project) (Marivoet et al., 2000; Pitsch and Beaucaire, 2000) by analysing variations in the hydrogeological system resulting from climate changes. This study takes account of the combined effects of variations in infiltration and sea level and the resulting erosion by rivers. Information on the extension of the ice sheet and the extent and thickness of permafrost are also taken into account.

Isotopic studies (stable isotopes and $^{14}C$) indicate that the dominant meteoric water component in these deep aquifers is up to 40,000 years old (Marivoet et al., 2000). Therefore the present-day system of aquifers has evolved over a considerable time span that is comparable with the assessment timescale. Pore water in the clay host rock is assumed to be relatively old, though the fact that it is fresh indicates that original depositional seawater has been largely displaced. Numerical modelling of the evolution of the aquifers has been carried out, using palaeohydrogeological boundary conditions, for example, enhanced hydraulic gradients due to influx of melt water run-off from the north European ice sheet (Marivoet et al. 2000). Results are generally consistent with the stable isotopic compositions and $^{14}C$ ages of present-day groundwaters.

The 'normal evolution' assessment model considers hydrogeological changes caused by climate changes, i.e. permafrost and glaciation. Although palaeohydrogeological information is not used explicitly in SAFIR-2 to constrain these potential future impacts, it is referred to as one of the multiple lines of reasoning for building confidence in hydrogeological simulations. Hydrochemical and isotopic studies are proposed as providing 'indications of the rate and possible evolutions of groundwater movement'. In effect, the most significant contribution with respect to PA is towards confirmation that water and solute transport through the Boom Clay throughout a 'normal evolution', in which hydraulic boundaries in adjacent aquifers will change, is fundamentally controlled and limited by diffusion.

The international peer review of SAFIR-2 remarks that research in PHYMOL into the implications of moderate glaciation for the normal evolution scenarios should be incorporated into future safety assessments in a structured way (NEA, 2003). Another review of SAFIR-2 by the Scientific Consultative Reading Committee considers that it is important to analyse the possible changes in groundwater movements caused by climate changes, i.e. by permafrost and glaciation or by global warming, and also the associated hydrogeochemical consequences (R38 in ONDRAF/NIRAS, 2001b).

The Reading Committee also comment that more attention should be given to the origin, age and change in chemistry of the interstitial water of the Boom Clay and surrounding aquifers, and that a palaeohydrogeological approach would be useful (R43 in ONDRAF/NIRAS, 2001b).

### A2.2 Opalinuston, Switzerland (Nagra, 2002a,b)

Palaeohydrogeology is an implicit part of characterisation of a claystone host rock because the entire host rock system is conditioned by water that is of considerable age. Evidence for the strong barrier-function of the Opalinus Clay within the surrounding system is derived from hydrochemical and isotopic data. Numerical analysis of how these have evolved shows that diffusion is the controlling transport process and that the solute and water system has not been perturbed by external forces (e.g. climate) for at least 250,000 years and possibly up to a million years. Over that time, the rate of advection has never exceeded $10^{-12}$ m/s (Nagra, 2002b). The preservation of unoxidised pyrite and siderite in the claystone is evidence that reducing conditions have persisted since deposition of the sediments. Hydrochemical and mineral data and their palaeohydrogeological interpretation show that the impact on groundwater of Quaternary surface evolution (periglacial conditions, river down-cutting and general erosion) has been attenuated so that the impact at 550m depth is undetectable.

As in Nagra's Kristallin-1 safety case, parameter uncertainty, e.g. in groundwater advection through the claystone host rock, is handled primarily by sensitivity analysis in the reference scenario. Some scenarios are considered as alternative conceptualisations and amongst these is the impact of glacial loading on the claystone (Nagra, 2002b). In this case, the claystone is assumed to remain unperturbed, with support for this coming from the palaeohydrogeology of clay pore waters which clearly shows that the six previous Quaternary cycles of glaciation have had no perceptible impact on the transport processes of solutes (Nagra, 2002a):

- Measured isotope and hydrochemical profiles from adjacent aquifers into the Opalinus Clay provide key data on the long-term large-scale transport properties of the clay;
- Measured isotope and hydrochemical profiles around faults intersected in the borehole at Benken and in the URL at Mont Terri show that the faults have not been active and have had no groundwater flow in them for considerable period of time;
- Groundwater ages from isotopic data are consistent with the timescales of modelled groundwater movement.

### A2.3 Yucca Mountain, USA (USDOE, 2000a)

Palaeohydrogeology is having a significant and visible role in the total system performance assessment (TSPA) of the proposed repository in a sequence of tuffaceous volcanic rocks of mid-Tertiary age at Yucca Mountain, Nevada, USA. The proposed repository's location is unique among spent fuel repository projects in that it will be in unsaturated rock, between 200-500m below the surface of Yucca Mountain and on average about 300m above the water table. The deep water table and very thick unsaturated zone are characteristic of the semi-arid present-day climate in this region.

Two scenarios linked to climate change for PA have been addressed by palaeohydrogeology: (i) potential rise of the water table, specifically whether it could ever rise to the proposed repository horizon, and (ii) future variations, maximum and minimum, of infiltration through the unsaturated sequence above and below the repository horizon. Palaeohydrogeological evidence is derived mainly from isotopic studies of water ages in the unsaturated (vadose) zone, in perched water tables, and in saturated zone groundwater beneath the water table, and from mineralogical and isotopic studies of fracture-filling minerals in the unsaturated zone.

The long-term average infiltration flux is supported by chloride mass balance (CMB) and by $^{14}C$ data for $CO_2$ in exchange equilibrium with unsaturated water at various depths, giving a time-averaged rate of movement in the past few thousands of years (USDOE, 2000b, 2001). Fracture minerals from the unsaturated zone have also been a major contributor to palaeohydrogeology (USDOE, 2000b; Vaniman and Chipera, 1996; Denniston et al, 1997; Neymark et al., 2000; Neymark and Paces, 2000; Neymark et al., 2001; Whelan et al., 2001; Wilson et al., 2001; Paces et al., 2001; Neymark et al., 2002; Whelan et al., 2002; Neymark et al., 2003; Whelan et al., 2003; Wilson et al., 2003; Paces et al., 2004; Gascoyne et al., 2002).

Coarse, sparry crystals of calcite and thin sheets or 'lacy' patchworks of opal have been precipitated on fracture surfaces and in lithophysal cavities. The opal deposits have quite high uranium, thorium and lead concentrations (typical ranges 20-150 ppm, 5-60ppm and 40-100 ppm respectively) that make small samples amenable to dating by $^{230}Th/^{234}U$ and $^{207}Pb/^{235}U$ methods. Calcite has been dated by $^{230}Th/^{234}U$ and also by $^{14}C$. Outermost layers of calcite and opal have age ranges from 16,000 to >500,000 years and are interpreted as the timing of slow mineral precipitation from percolating water films. Heterogeneity of ages at a small (micrometre) scale indicates that minerals have grown unevenly and have sector zoning as well as concentric zoning. In general, inner layers have older $^{230}Th/^{234}U$ ages indicating progressive outward growth (<5mm of mineral per million years). $^{18}O/^{16}O$ and $^{13}C/^{12}C$ variation in calcite are in the ranges +10 to +21‰ $\delta^{18}O_{SMOW}$ and -8.2 to +8.5‰ $\delta^{13}C_{PDB}$ with the oldest calcite having higher $\delta^{13}C$ and lower $\delta^{18}O$. $^{87}Sr/^{86}Sr$ was also measured, older calcite correlating with the isotopic composition of tuff whilst younger calcite has higher more radiogenic $^{87}Sr/^{86}Sr$. Overall, the isotopic data for ages and depositional environments have been interpreted as providing a record of continuous stable infiltration of meteoric water through a limited network of connected fracture pathways (only ca. 6% of fractures) for at least the last million years (Wilson and Cline, 2001; Whelan et al., 2001; Wilson et al., 2003)

Calcite from older parts of the mineral coatings contains some two-phase fluid inclusions that give homogenisation temperatures of 30-85ºC, as well as single-phase liquid inclusions. These data, together with $\delta^{18}O$ data for the host calcite, have led to a hypothesis of upwelling hydrothermal waters in the past (Dublyansky, 2001, 2002; Dublyansky et al., 2001, 2004). However this hypothesis was rejected by Whelan et al. (2001), Wilson et al. (2003) and Neymark et al. (2001) who reconciled the $T_h$ and $\delta^{18}O$ data with fluid inclusion entrapment and calcite deposition in the early stages of infiltration into a cooling volcanic rock mass.

Palaeoclimatic interpretation for the region around Yucca Mountain over the last 5,000,000 years is supported in remarkable detail by the stable isotopic ($^{18}O/^{16}O$) variations in vein calcite that has accumulated in an open fault (Devil's Hole) adjacent to a groundwater discharge area in south-central Nevada (Winograd et al., 1992). Groundwater transit times from recharge to discharge at Devil's Hole are several thousands of years, indicating that the $\delta^{18}O$ signal in vein calcite is likely to be a good archive of temporal variations in the $\delta^{18}O$ of precipitation at the recharge area which reflect changes in temperature as well as changes in isotopic composition of the moisture source (i.e. oceanic sources). The chronology of calcite accumulation was calibrated by $^{230}Th/^{234}U$ dating (and later supported by $^{231}Pa$ dating; Edwards et al., 1997), and the $\delta^{18}O$ variations correlate fairly well with climate-driven fluctuations in the marine sedimentary record and Antarctic ice cores through several glacial stages.

# Appendix B: Application of ESL

## B1 INTRODUCTION

In 2004, Nirex invited Quintessa to undertake a demonstration of the potential application of Evidential Support Logic (ESL), as a contribution to PADAMOT, with the aim of providing a structured logical analysis of the use of palaeohydrogeological evidence in support of site evaluation and safety case development. Specifically, ESL was to be used to determine the degree of support for the statement that "environmental change at the surface has little impact at repository depth".

In the following Sections B2 and B3, the general principles behind the use of ESL are described, whilst in Sections B4 and B5 the technique is applied to palaeohydrogeological evidence from Sellafield and the results are presented.

## B2 ESL: A TOOL FOR STRUCTURED USE OF DATA

ESL is a methodology for assembling evidence from diverse sources in a coherent decision support model (Bowden, 2004; Metcalfe et al., 2002; Seo et al., 2004). It formalises and makes transparent the subjective processes of expert judgment that are inherent in drawing general conclusions from detailed supporting evidence, taking account of the sources and implications of uncertainty. ESL involves three main steps (Bowden, 2004):

1. Development of a hierarchical process model to provide a common, coherent logical structure for assembling all the evidence that is relevant to an identified top-level process or hypothesis;
2. Parameterisation of the model and identification of sources of evidence that contribute arguments for and/or against sub-processes in the logical model; and
3. The propagation of evidence through the process model, representing uncertainty using the principles of Interval Probability Theory (IPT), to provide an assessment of the dependability of the overall top-level process.

ESL involves appraising the support provided from a number of sub-processes ('child' processes) for an identified top-level ('parent') process of interest. A process hierarchy links the top-level process to data at the lowest level, usually via intermediate steps, or sub-processes. In the PADAMOT exercise, the top-level process is a logical and defensible appraisal of a hypothetical scenario that might be significant in Performance Assessment – for example, assessment of the hydrogeological impact of future glaciation based on evidence from palaeohydrogeological methods such as hydrogeochemistry and mineralogy.

The hierarchical model comprises a top-down decomposition of the various factors that contribute to a process until a level of detail is reached at which experts are comfortable to make direct judgments about the level of support that available evidence provides for and against the sub-process. The software tool TESLA (The Evidence Support Logic Application; Quintessa Ltd) was used to visualise the hierarchical structure of processes and then to use IPT to propagate evidence and uncertainties through the hierarchy to arrive at logical decisions.

IPT uses three-value logic to assess uncertainty as well evidence for and against a process or proposition, i.e. a probability summation: evidence for + evidence against + uncertainty = 1. This is illustrated in Figure B1, in which evidence for is represented as green, evidence against as red, and residual uncertainty is white. With the three-value formalism, evidence for and evidence against can be evaluated independently, each ranging from 0 to 1, with uncertainty taking a value from -1 to +1. An uncertainty of 1 implies that there is no evidence at all on which to base a judgment, whereas a negative value indicates a situation in which the assessed evidence for and against total more than 1; that is to say, a situation in which the evidence is in conflict.

The fundamental approach to the propagation of evidence using IPT is based on a combination of evidence whereby the result is always greater than (or equal to) the largest contributing evidence value. The effect is additive (though not linearly additive), such that two separate lines of evidence that both support (or refute) a hypothesis reinforce each other such that their combined evidence is more supportive than either piece of evidence taken individually. The combination of evidence is modified by three factors: *sufficiency*, *dependency* and *necessity*.

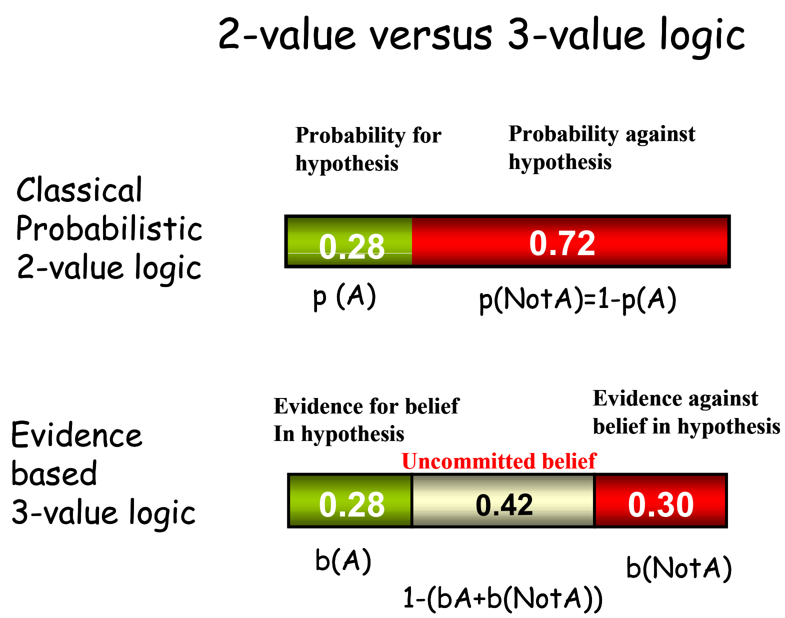


**Figure B-1. Classical two-value probabilistic analysis compared with three-value interval analysis**

At every branch within the hierarchical process model, each sub-process (child process) is assigned a **sufficiency** that dictates how much weight should be given to it when determining the combined evidence of its parent process. The sufficiency of a sub-process represents its overall relevance to making a judgment about the dependability of the higher level process. The sufficiency parameter can take a value between 0 (insufficient) and 1 (completely sufficient) – a greater level of sufficiency results in evidence values associated with the sub-process being propagated more strongly up the hierarchy.

Within each set of sub-processes at a given level in the process model hierarchy, there is a chance that some of the information may be overlapping, or shared. This is reflected by setting a **dependency** parameter to describe the assumed degree of commonality between contributing processes and to avoid double counting the support that is provided by mutually dependent pieces of evidence. The dependency parameter may take a value between 0 (completely independent) and 1 (completely dependent).

Sub-processes that are necessary for the success of the parent process, i.e. which upon failure will necessarily lead to failure of the higher level process are indicated by a Boolean operator **necessity**: it is set at TRUE if the process is necessary and FALSE otherwise.

## B3 ELICITING EVIDENCE AND ASSESSING UNCERTAINTIES

Qualitative judgments of evidence are elicited from suitably qualified experts in terms of 'evidence for' and 'evidence against' the dependability of each lowest-level sub-process. These are subsequently converted to numbers with TESLA. Contributions to uncertainty come from: incomplete knowledge of process and of the system, uncertain quality or meaning of data, conflict and/or variability in data.

Two main steps are followed in characterising uncertainty. First, the adequacy of the experts' knowledge base was assessed. Then judgments are made of the 'face value' and quality of available evidence in support of (or against) the process in question. The net value of the evidence is determined by first selecting a value function that reflects judgment of the face value of that evidence. The appropriate location of that value function is then determined by assigning a degree of confidence in the quality of the available evidence.

In the geological context, the indicators of quality are familiar confidence building measures used in the peer review process e.g. theoretical basis, scientific method, auditability, calibration, validation and objectivity (Bowden, 2004). For each process for which evidence is input, scores for the supporting and refuting evidence are elicited based on the various quality indicators.

Within the TESLA software tool, the propagation of 'evidence for' is treated independently from that for 'evidence against', using standard probability theory. A simple illustration of the parameterisation procedure for the propagation of evidence and uncertainty is shown in Figure B2.

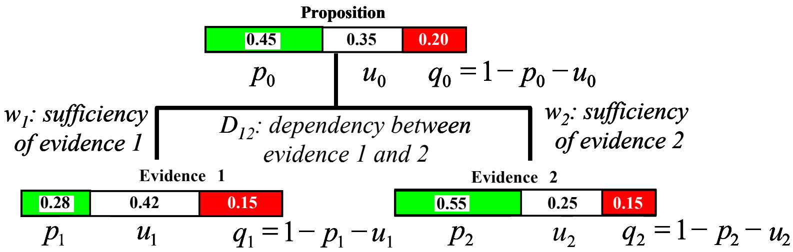


**Figure B2. Propagation of uncertainty in a process model. The minimum probabilities that some evidence supports or refutes a proposition are given by p and q and u is the residual uncertainty.**

The implementation of Evidence Support Logic for the current study was carried out with the support of the TESLA software tool. An important facility of TESLA for the current study was the *tree view* decision display. An example of this, representing a segment from one of the outputs generated during the course of the current work, is shown in Figure B3.

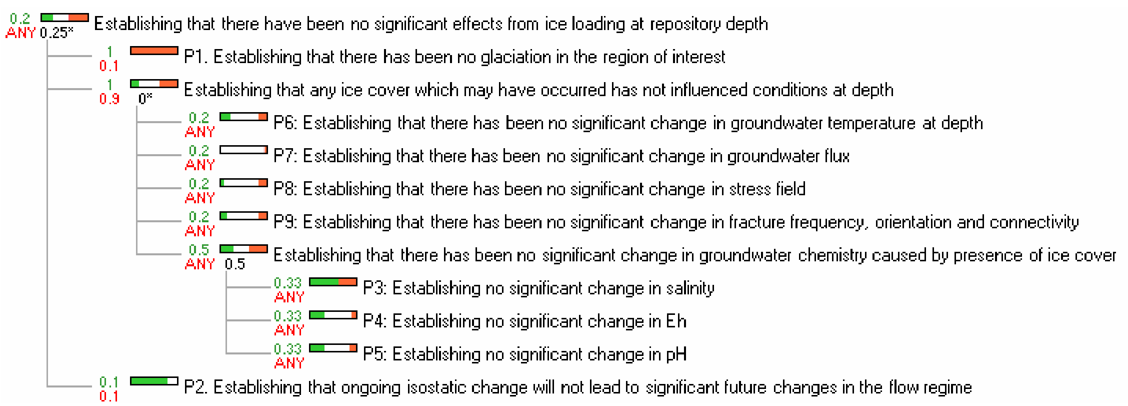


**Figure B3. Example of ESL visualisation in the TESLA 'tree view' display**

Evidence information about a process in the ESL model is displayed graphically using the ‘Italian flag’ representation described earlier. Numeric values for *sufficiency* are shown to the left of the evidence display bar for each sub-process in the model. ‘Sufficiency for’ and ‘sufficiency against’ are coloured green and red, respectively. ‘ANY’ is shown where the success or failure of <u>any</u> (and every) sub-process can be sufficient on its own to ensure the success or failure of the parent. ‘ALL’ is shown where <u>all</u> the sub-processes are required to ensure success (or failure) of the process. If an individual sub-process is deemed to be a *necessity*, then the background to the display icon for that particular sub-process is shaded grey. Values of the assigned *dependency* parameter are displayed in the tree view beneath the evidence display bar for each parent process. The numeric value shown corresponds to whatever is the assumed ‘general dependence’ between the identified sub-processes.

Using the TESLA software tool, two main approaches to visualising outputs from an ESL analysis have been devised: the Evidence-ratio plot and the sensitivity (or Tornado) plot (Bowden, 2004).

The Evidence-ratio Plot (Figure B4) illustrates the levels of evidence relating to each right-most child process in the hierarchical model (or sub-element of the model) as in Figure B3. The horizontal axis indicates the percentage uncertainty in the evidence, or alternatively that fraction of the total available belief which is assigned to an uncommitted state. An increasing negative value along the horizontal axis represents the existence of increasing conflict in the evidence. The vertical axis indicates the ratio of ‘evidence for’ to ‘evidence against’ associated with each process.

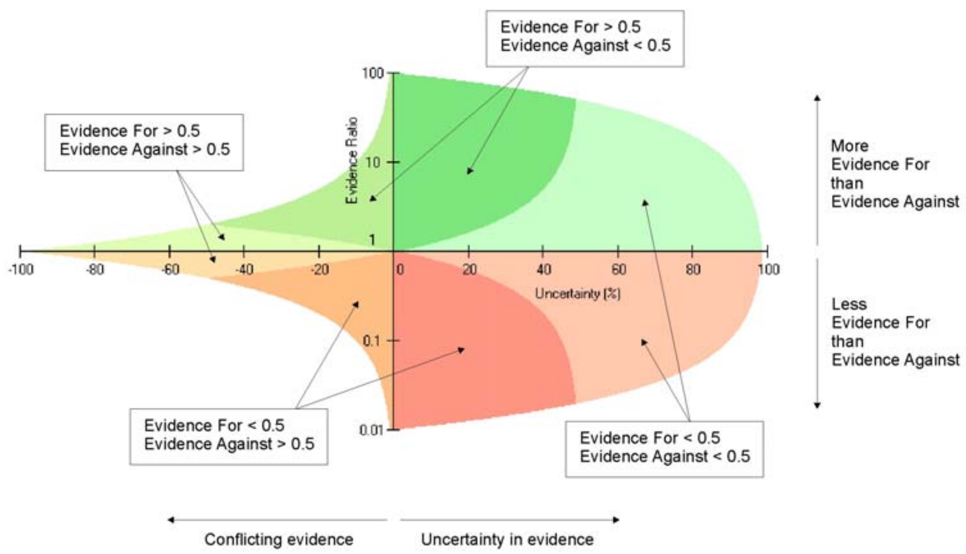


**Figure B4. Regions of the Evidence-ratio Plot.**

The Tornado, or sensitivity, Plot considers only the right-most child processes in an ESL model (or section of such a model) (Figure B5). Its function is to indicate the impact that each of these sub-processes has on the overall decision; that is to say, how much a small change in evidence for a process will influence the calculated support for the top process.

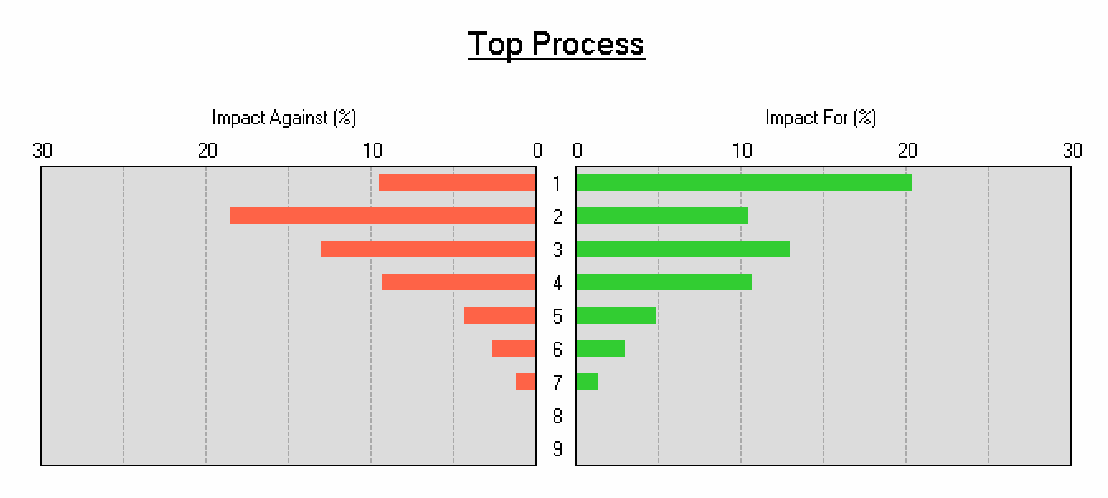


**Figure B5. Example Tornado Plot; each of the numbered horizontal bars, 1 to 9, represents a right-most child process (see Figure B3) and indicates its relative impact for and against the decision on the top-level process.**

## B4 APPLICATION TO PALAEOHYDROGEOLOGICAL EVIDENCE

The Expert Group comprised members from UK partners in PADAMOT (Nirex, BGS, Intellisci) and Quintessa. The overall aim was to investigate whether ESL could be used to rationalise the use of palaeohydrogeological information to constrain scenarios that need to be considered in a safety case.

The work was divided into two main parts: (i) The development of a generic ESL model structure for assessing the support that might be provided by palaeohydrogeological evidence to the top-level hypothesis that environmental change at the surface has little impact at repository depth; (ii) The implementation of a scenario-specific version of the generic model, focusing on application to the Sellafield site for which relevant data have been acquired in PADAMOT and the preceding project EQUIP.

It was not possible to use all of the techniques described above in the PADAMOT study because of the limited scope and resources; therefore the analysis here is an illustrative but incomplete demonstration of ESL.

Two aspects of the top-level hypothesis were important in developing, implementing and interpreting the ESL model. First, the evidence was being evaluated against a negative statement or 'null hypothesis', i.e. evidence *against* the hypothesis is evidence *supporting* the demonstration that significant change in repository evolution can take place. Secondly, the meaning of ‘change’ at depth was interpreted separately for each of the lowest level sub-processes in the model.

There are two alternative ways to define a model structure in this case: a 'EFEPs-based' model and a 'System Properties' model. Both were attempted in this trial of the ESL methodology.

The **'EFEPs-based' model** bases its logical structure (see Figure B6) on the influences of external (i.e. environmental) features, events and processes (EFEPs). It is an understandable approach because it is standard practice to evaluate scenarios for system evolution by screening EFEPs. The ESL model can, in theory, be made comprehensive by representing all potentially relevant EFEPs associated with surface environmental change in the model structure. Palaeo-evidence is then examined to consider whether or not it supports the case for the action of those EFEPs. However the underlying evidence for change does not necessarily allow an easy distinction to be made between the potential causes of that change, so there will be considerable dependency within the model with duplication in the sources of evidence used to evaluate support for, or against, a range of different EFEPs. At the same time, the strength of the available evidence, in terms of its sufficiency, tends to be reduced, in so far as the existence of evidence for a particular type of change cannot necessarily be taken as unique evidence for the action of a specific EFEP.

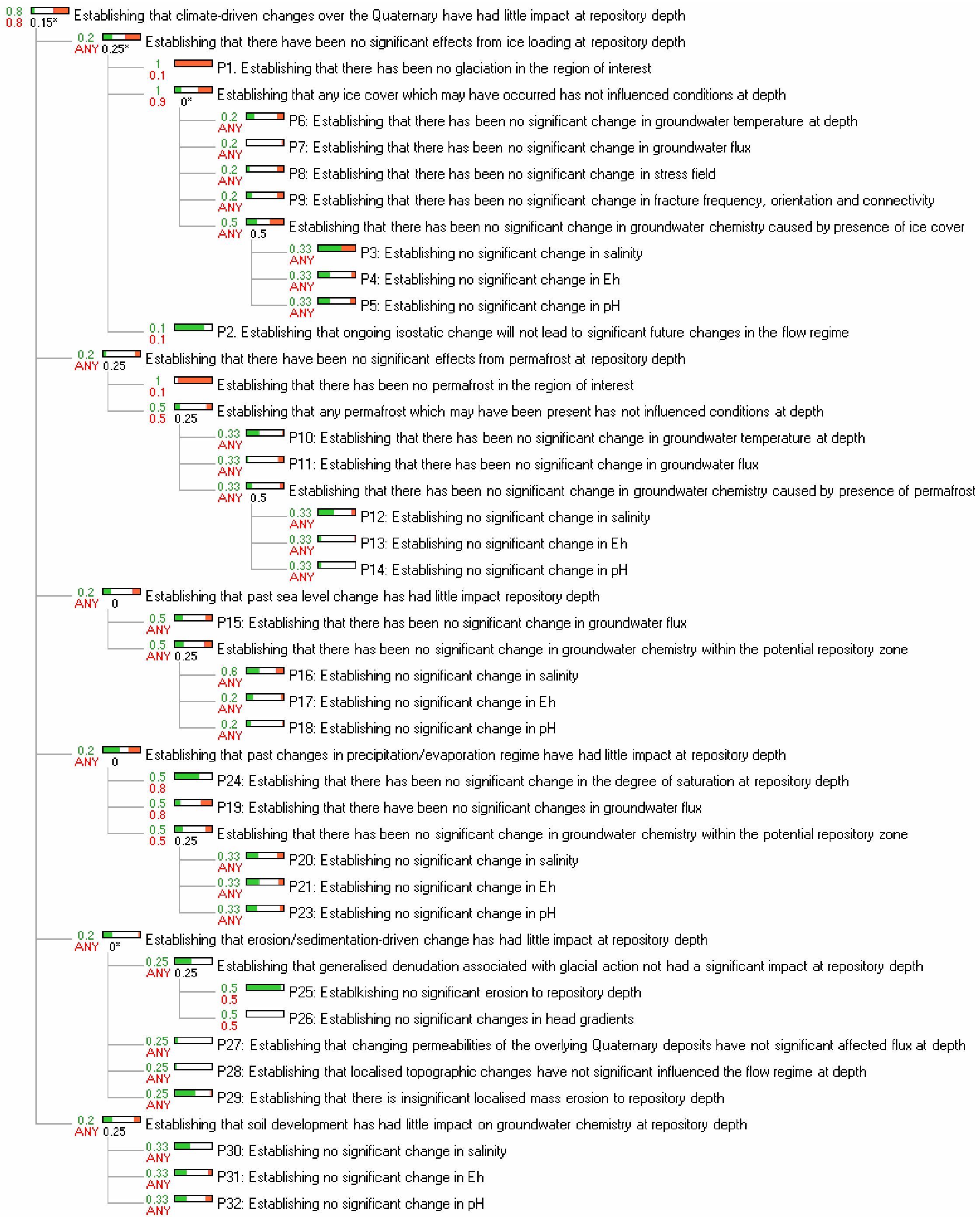


**Figure B6. Structure, sufficiency parameters and propagated evidential judgments for the Sellafield-specific application of the EFEPs-based Model.**

For possible climate-driven environmental change, an initial sub-division is made into two sub-processes: one concerning the palaeohydrogeological evidence of changes during the Quaternary period and one concerning the comparability of future changes (i.e. scenarios) with those in the past. Sub-processes of possible past change relate to the effects of ice loading, permafrost, eustatic sea level change, precipitation/evaporation regime, erosion/sedimentation processes and soil development. The detailed expansion of the process model down to the basic child processes illustrates the degree of potential redundancy that exists in the model. For example, information relating to changes in groundwater chemistry is relevant to assessing the potential evidence of all climate change EFEPs except for erosion/sedimentation. Therefore there is a high degree of dependency between these different sub-processes. The logical structure of the ESL model exposes the interpretative challenges that are faced in making expert judgments and makes transparent the implications that are drawn from the available evidence.

The somewhat simpler **'System Properties' model** ignores the potential causes of change in the first instance and develops a process hierarchy based directly on evidence for changes in system properties (see Figure B7). Although simpler, the outcome cannot so easily be tied to the process of scenario development since there is no explicit relation between the results of the evidence evaluation and underlying EFEPs except at the lowest level of the model where the sub-processes identify potential causes of changes in rock system properties.

Parameterisation of the alternative ESL models would have involved quantifying the values for *sufficiency*, *dependence* and *necessity* at every branch in the two models. However time constraints on the application of ESL for PADAMOT meant that it was not possible to undertake this component of the exercise via a formal elicitation. Instead, parameter values were assigned by Quintessa using in-house expert judgment and subsequently presented to the Expert Group for review.

The parameterisation of the EFEPs-based model is shown in Figure B6. Some aspects to note are:

- Because the structure of the model is derived from a top-level process that is a null hypothesis, then at several levels it is sufficient for only one of the sub-processes to be capable of refuting the parent process in order to ensure the failure of that process.
- In many cases, it is less easy to quantify the sufficiency of sub-processes in terms of their potential support for a given process. As a general rule, many sub-processes have a comparatively low value of sufficiency for support of the parent process. A useful approach for setting sufficiencies is to consider (i) the degree to which the success of all the child processes of a given parent would be sufficient to guarantee the success of the parent, and (ii) the relative importance (sufficiencies) of the different sub-processes. In some cases, it can be helpful to structure the model so that as far as possible the child processes of a given parent process are all roughly of equal significance.
- Establishing appropriate dependency values is not simple. In some cases, it has been assumed that there is a generic dependency in the region of 25% between sub-processes, reflecting the judgment that there is a measure of shared information. Elsewhere, a general dependency of zero has been assumed (i.e. assuming that the sub-processes are completely independent), sometimes with a few selected sub-processes being assigned a much stronger dependency. A useful approach is to structure a model so that dependencies are minimised
- There is an assumed strong dependence between many of the sub-processes to the parent process of '*Establishing that climate-driven changes over the Quaternary have had little impact at repository depth*'. This dependency arises because much of the information used to define evidence in favour or against these sub-processes is shared and there is little information to distinguish between the EFEPs that were responsible for that change.

The parameterisation of the System Properties model is illustrated in Figure B7. In many cases, the assigned sufficiency and dependency values have been left at their default values (sufficiency = 0.5, dependency = 0). Elsewhere, the basic principles underpinning the parameterisation of the System Properties process model (including the definition of the top-level process in terms of a null hypothesis) are broadly similar to those associated with the EFEPs model.

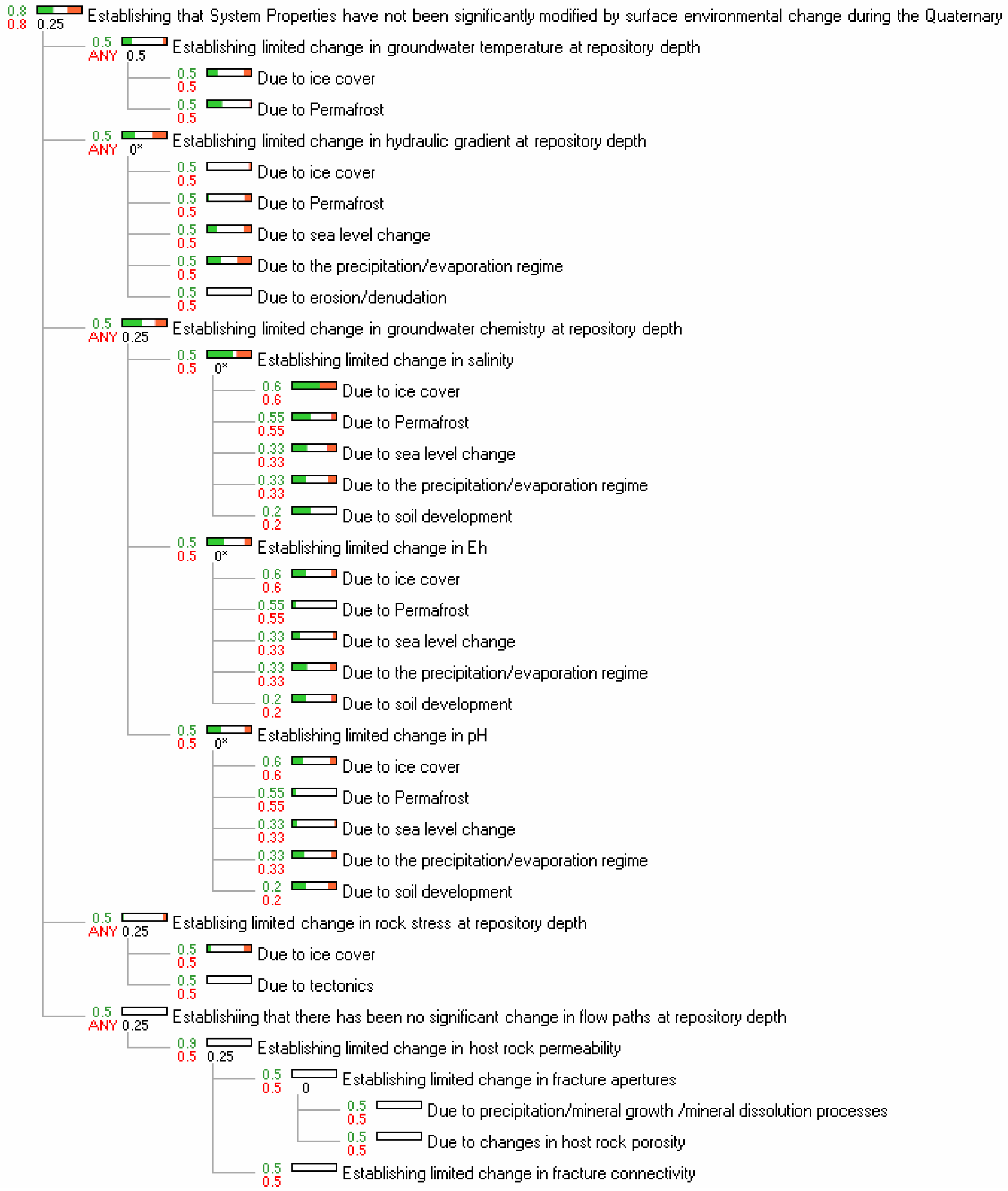


**Figure B7. Structure, sufficiency parameters and propagated evidential judgments for the Sellafield-specific application of the System Properties Model.**

As noted at the outset, one of the limitations of the current study was the fact that it was established with the primary aim of illustrating the potential for information derived from palaeohydrogeological studies to be used systematically in support of the development of a performance assessment for deep geological disposal of radioactive waste. As is evident from the structure of the generic models, such evidence needs to be used alongside other types of evidence as part of a comprehensive structured evaluation of the top-level hypothesis. Therefore the quantitative implementation of the model was focused on sub-branches of the two ESL models, where most effective use could be made of palaeohydrogeological data and other aspects of the evolution of systems for water-rock interactions. In the case of the EFEPs-based model, that meant focusing on the sub-branch for which the top-level process is '*Establishing that climate-driven changes over the Quaternary have had little impact at repository depth*', while for the Process System model, the equivalent new top-level process became '*Establishing that System Properties have not been significantly modified by surface environmental change during the Quaternary*'.

## B5 RESULTS AND CONCLUSIONS FROM THE APPLICATION OF ESL

### B5.1 EFEPs-based model

The full description of the basic child processes, the corresponding critical success factors and the relevant Sellafield-specific sources of evidence that are relevant to the sub-branch being considered in the EFEPs model ('*Establishing that climate-driven changes over the Quaternary have had little impact at repository depth*') are given in Egan and Bowden (2004). Judgments of many of the sub-processes rely on sources of evidence that are outside the scope of PADAMOT. Nevertheless, an illustrative selection of critical success factors and sources of information for the basic child processes that specifically use palaeo-hydrogeological data and interpretation acquired in PADAMOT are given below[1]:

P3 Establishing no significant change in groundwater salinity at depth as a result of the presence of ice cover

> Critical success factor: The process will be considered successful if: (a) it is demonstrated that the freshwater-saline interface has not moved across the PRZ (significant vertical movement); (b) it is demonstrated that salinity at repository depth has not increased from current levels to those characteristic of the basinal brines (lateral movement of the brine/saline front).
>
> Relevant sources of information: fluid inclusion chemistry, calcite morphology and growth zoning, groundwater chemistry, mineral assemblage, mineral corrosion, spatial distribution of groundwater composition, modelling.

P4 Establishing no significant change in groundwater redox conditions at depth as a result of the presence of ice cover

> Critical success factor: The process will be considered successful if it is demonstrated from the available evidence that changes in redox conditions at repository depth are always reducing (in terms of maintaining Fe, Mn, and redox-sensitive radionuclides in their reduced forms).
>
> Relevant sources of information: groundwater chemistry, mineral assemblage, mineral composition/growth zoning, mineral oxidation/reduction, spatial distribution of mineralization, spatial distribution of groundwater composition, modelling, carbon & sulphur isotope composition, organic composition in groundwater.

P5 Establishing no significant change in groundwater pH at depth as a result of the presence of ice cover

> Critical success factor: The process will be considered successful if it is demonstrated from the available evidence that changes in ambient pH at repository depth are within a range 6 to 9.
>
> Relevant sources of information: groundwater chemistry, mineral assemblage, mineral composition/growth zoning, mineral corrosion, spatial distribution of mineralization, spatial distribution of groundwater composition, modelling.

P6 Establishing that there has been no significant change in groundwater temperature at depth as a result of the presence of ice cover

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[1] The numbering scheme relates to Figure B6.

Critical success factor: The process will be considered successful if it is demonstrated from the available evidence that there has been no groundwater freezing at repository depth (not concerned with upper bound temperatures because these will be outside the range associated with surface-driven environmental change).

Relevant sources of information: modelling of geothermal gradient of heat flux within Quaternary context, groundwater cation ratios/fluid inclusion salinity, mineral fluid inclusion closing temperature.

P7 Establishing that there has been no significant change in groundwater flux at depth as a result of the presence of ice cover

Critical success factor: The process will be considered successful if it is demonstrated from the available evidence that there has been no reversal of groundwater flow.

Relevant sources of information: isotopic composition of groundwaters indicative of glacial recharge, dissolved gas content in groundwaters, general chemical composition of groundwaters, mineral growth history, mineral dissolution and secondary porosity formation with related precipitation and sealing, in situ pressure measurements, relics of glacier induced flow structures e.g. eskers, tunnel valleys, modelling of hydraulic gradient under ice loading.

P10 Establishing that there has been no significant change in groundwater temperature at depth as a result of the presence of permafrost

Critical success factor: as P6.

Relevant sources of information: modelling of geothermal gradient, depth of permafrost and associated heat flux within Quaternary context, groundwater cation ratios/fluid inclusion salinity, mineral fluid inclusion closing temperature, stable isotopic composition of calcite, freezing-induced precipitation of minerals.

P11 Establishing that there has been no significant change in groundwater flux at depth as a result of the presence of permafrost

Critical success factor: as P7.

Relevant sources of information: isotopic composition of groundwaters indicative of permafrost effects, dissolved gas content in groundwaters, general chemical composition of groundwaters, mineral growth history, mineral dissolution and secondary porosity formation with related precipitation and sealing, in situ pressure measurements.

P12 Establishing no significant change in groundwater salinity at depth as a result of the presence of permafrost

Critical success factor: as P3.

Relevant sources of information: as P3.

P13 Establishing no significant change in groundwater redox conditions at depth as a result of the presence of permafrost

Critical success factor: as P4.

Relevant sources of information: as P4.

P14 Establishing no significant change in groundwater pH at depth as a result of the presence of permafrost

Critical success factor: as P5.

Relevant sources of information: as P5.

P15 Establishing that there has been no significant change in groundwater flux at depth as a result of past sea level change

Critical success factor: as P7.

Relevant sources of information: isotopic composition of groundwaters indicative of permafrost effects, dissolved gas content in groundwaters, general chemical composition of groundwaters, mineral growth history, mineral dissolution and secondary porosity formation with related precipitation and sealing, in situ pressure measurements.

P16 Establishing no significant change in groundwater salinity at depth as a result of past sea level change

Critical success factor: as P3

Relevant sources of information: as P3

P17 Establishing no significant change in groundwater redox conditions at depth as a result of past sea level change

Critical success factor: as P4.

Relevant sources of information: as P4.

P18 Establishing no significant change in groundwater pH at depth as a result of past sea level change

Critical success factor: as P5.

Relevant sources of information: as P5.

P19 Establishing that there has been no significant change in groundwater flux at repository depth as a result of changes in the precipitation/evaporation regime

Critical success factor: as P7.

Relevant sources of information: isotopic composition of groundwaters, dissolved gas content in groundwaters, general chemical composition of groundwaters, mineral growth history, mineral dissolution and secondary porosity formation with related precipitation and sealing, in situ pressure measurements.

P20 Establishing no significant change in groundwater salinity at depth as a result of changes in the precipitation/evaporation regime

Critical success factor: as P3.

Relevant sources of information: as P3.

P21 Establishing no significant change in groundwater redox conditions at depth as a result of changes in the precipitation/evaporation regime

Critical success factor: as P4.

Relevant sources of information: as P4.

P23 Establishing no significant change in groundwater pH at depth as a result of changes in the precipitation/evaporation regime

Critical success factor: as P5.

Relevant sources of information: as P5.

P27 Establishing that changes in permeabilities of the overlying Quaternary deposits have not significantly affected flux at depth as a result of erosion/sedimentation driven change

Critical success factor: as P7.

Relevant sources of information: as P19.

P30 Establishing no significant change in groundwater salinity at depth as a result of soil development

Critical success factor: as P3.

Relevant sources of information: as P3.

P31 Establishing no significant change in groundwater redox conditions at depth as a result of soil development

Critical success factor: as P4.

Relevant sources of information: as P4.

P32 Establishing no significant change in groundwater pH at depth as a result of changes in the precipitation/evaporation regime

Critical success factor: as P5.

Relevant sources of information: as P5.

The elicited evidence judgments were entered into the ESL software tool resulting in the parameterised EFEPs-based model shown in Figure B6. Some aspects to note are:

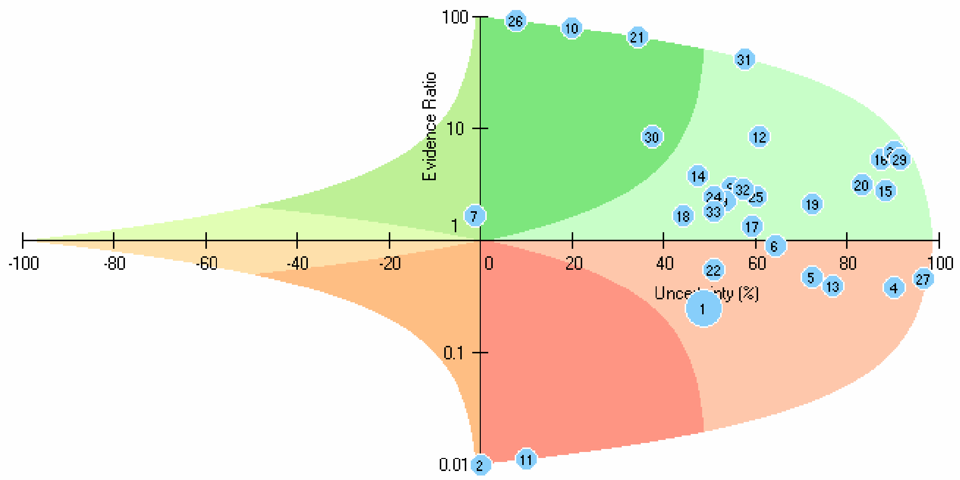
- Because the structure of the model is derived from a top-level process that is a null hypothesis, then at several levels it is sufficient for only one of the sub-processes to be capable of refuting the parent process in order to ensure the failure of that process.
- In many cases, it is less easy to quantify the sufficiency of sub-processes in terms of their potential support for a given process. As a general rule, many sub-processes have a comparatively low value of sufficiency for support of the parent process.
- Establishing appropriate dependency values is not simple. In some cases, it has been assumed that there is a generic dependency in the region of 25% between sub-processes, reflecting the judgment that there is a measure of shared information. Elsewhere, a general dependency of zero has been assumed (i.e. assuming that the sub-processes are completely independent), sometimes with a few selected sub-processes being assigned a much stronger dependency.

There is an assumed strong dependence between many of the sub-processes to the parent process of '*Establishing that climate-driven changes over the Quaternary have had little impact at repository depth*'. This dependency arises because much of the information used to define evidence in favour or against these sub-processes is shared and there is little information to distinguish between the EFEPs that were responsible for that change.

An Evidence-ratio Plot for the model is provided in Figure B8, and the corresponding Tornado Plot is shown in Figure B9. The results indicate that there is rather stronger evidence against the hypothesis '*that climate-driven changes over the Quaternary have had little impact at repository depth'* than there is in favour. The residual uncertainty is significant at approximately 50% and the overall evidence ratio for the hypothesis is not particularly large.

The Tornado plot shows that the most significant impact on uncertainty in the overall result is associated with the sub-process '*Establishing no significant change in groundwater salinity at depth as a result of the presence of ice cover*'. The main decision plot links this with the 'evidence against' this sub-process being propagated strongly through the model, due to the assigned sufficiency values. There is also some conflict in the input evidence, with limited residual uncertainty.

It should be noted that these conclusions do not represent unequivocal judgments about the Sellafield site or about the quality of data, as the ESL exercise is illustrative only. Rather it highlights areas where further research could usefully be targeted either to refine the model or to better demonstrate the relevance and quality of the underlying processes.




1 : Establishing that climate-driven changes over the Quaternary have had little impact at repository depth
2 : P1. Establishing that there has been no glaciation in the region of interest
3 : P6: Establishing that there has been no significant change in groundwater temperature at depth
4 : P7: Establishing that there has been no significant change in groundwater flux
5 : P8: Establishing that there has been no significant change in stress field
6 : P9: Establishing that there has been no significant change in fracture frequency, orientation and connectivity
7 : P3: Establishing no significant change in salinity
8 : P4: Establishing no significant change in Eh
9 : P5: Establishing no significant change in pH
10 : P2. Establishing that ongoing isostatic change will not lead to significant future changes in the flow regime
11 : Establishing that there has been no permafrost in the region of interest
12 : P10: Establishing that there has been no significant change in groundwater temperature at depth
13 : P11: Establishing that there has been no significant change in groundwater flux
14 : P12: Establishing no significant change in salinity
15 : P13: Establishing no significant change in Eh
16 : P14: Establishing no significant change in pH
17 : P15: Establishing that there has been no significant change in groundwater flux
18 : P16: Establishing no significant change in salinity
19 : P17: Establishing no significant change in Eh
20 : P18: Establishing no significant change in pH
21 : P24: Establishing that there has been no significant change in the degree of saturation at repository depth
22 : P19: Establishing that there have been no significant changes in groundwater flux
23 : P20: Establishing no significant change in salinity
24 : P21: Establishing no significant change in Eh
25 : P23: Establishing no significant change in pH
26 : P25: Establkishing no significant erosion to repository depth
27 : P26: Establishing no significant changes in head gradients
28 : P27: Establishing that changing permeabilities of the overlying Quaternary deposits have not significant affected flux at depth
29 : P28: Establishing that localised topographic changes have not significant influenced the flow regime at depth
30 : P29: Establishing that there is insignificant localised mass erosion to repository depth
31 : P30: Establishing no significant change in salinity
32 : P31: Establishing no significant change in Eh
33 : P32: Establishing no significant change in pH

**Figure B8. Evidence-ratio plot for the Sellafield-specific application of a selected branch of the EFEPs-based Model**

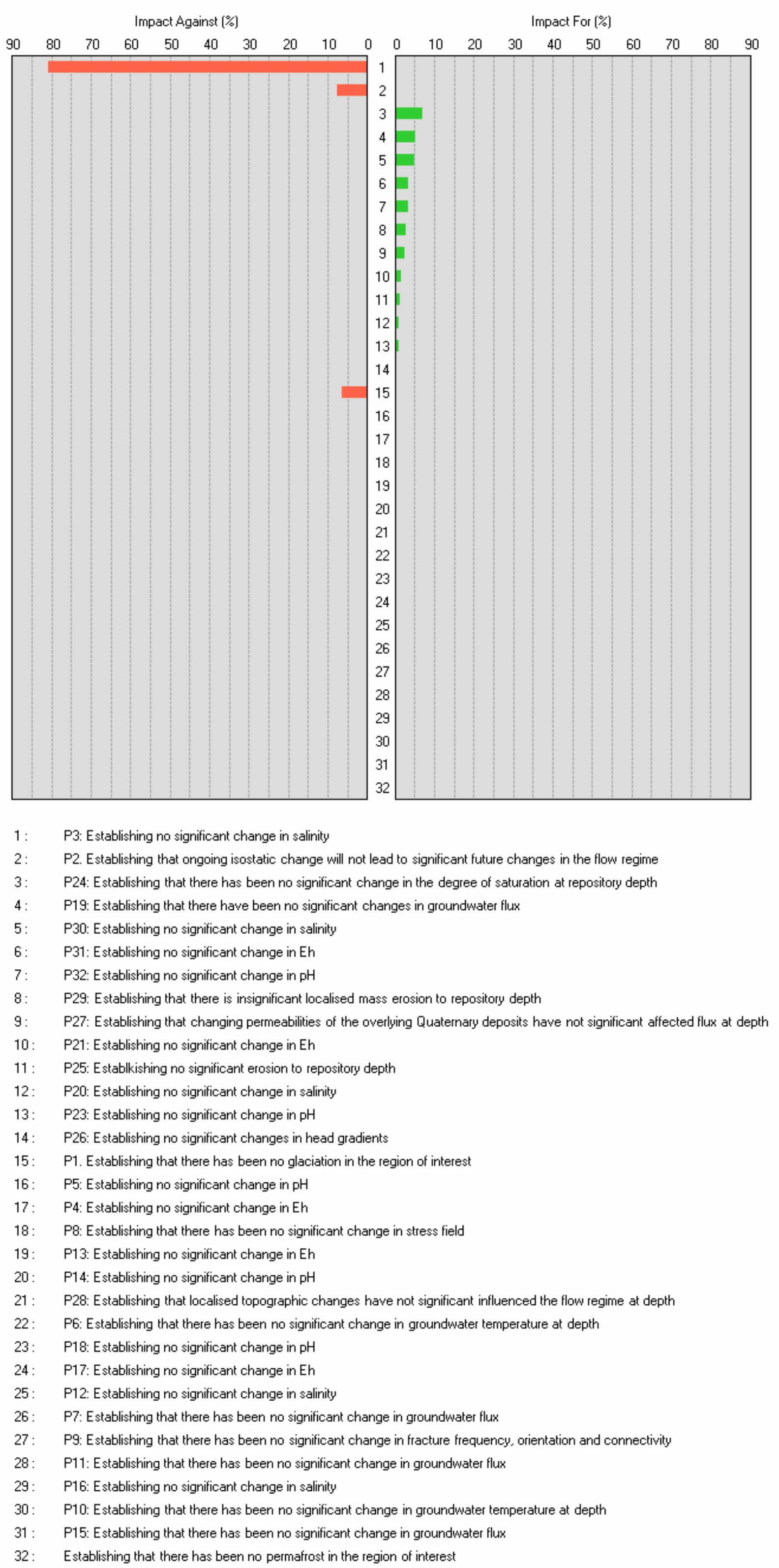
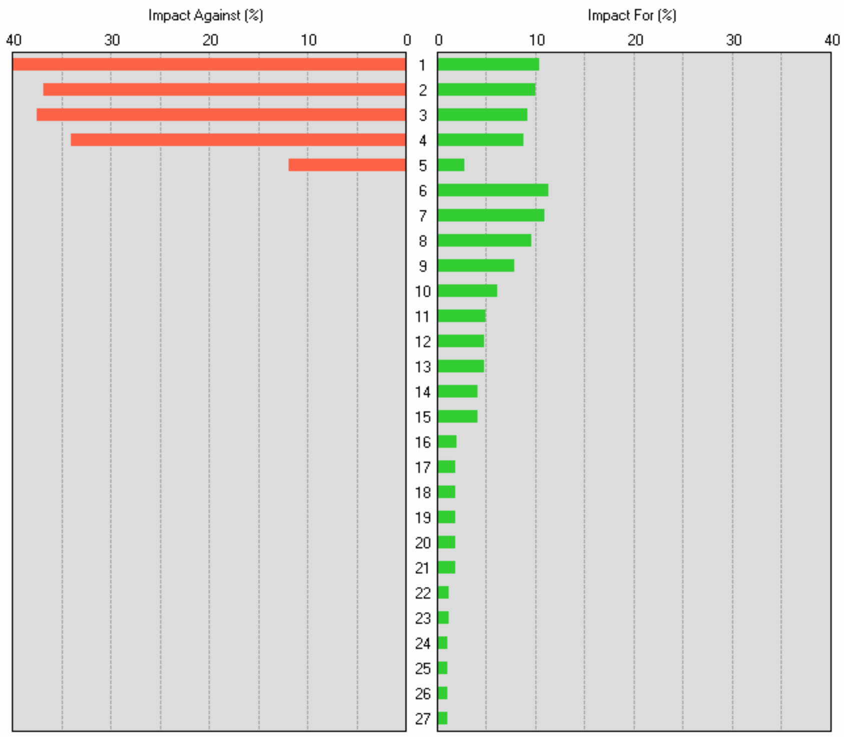



**Figure B9. Tornado plot for the Sellafield-specific application of a branch of the EFEPs-based Model**

### B5.2 System Properties model

It was not possible within the scope of the study to conduct a model-specific elicitation procedure for the System Properties ESL Model. Instead, for illustrative purposes, the responses from the evidence judgments for the EFEPs model were transferred directly into the System

Properties model shown in Figure B7. The results are shown as a Tornado Plot in Figure B10 and the Decision and Evidence-ratio plots are in Egan and Bowden (2004). The overall results are largely similar in quality to those obtained using the EFEPs model, indicating that there is evidence both for and against the hypothesis *'that System Properties have not been significantly modified by surface environmental change during the Quaternary'*. The residual uncertainty is quite large and the overall evidence ratio for the hypothesis is close to unity.




1 : Due to the precipitation/evaporation regime
2 : Due to sea level change
3 : Due to Permafrost
4 : Due to erosion/denudation
5 : Due to ice cover
6 : Due to Permafrost
7 : Due to ice cover
8 : Establishing limited change in fracture connectivity
9 : Due to tectonics
10 : Due to ice cover
11 : Due to ice cover
12 : Due to precipitation/mineral growth /mineral dissolution processes
13 : Due to changes in host rock porosity
14 : Due to ice cover
15 : Due to ice cover
16 : Due to the precipitation/evaporation regime
17 : Due to the precipitation/evaporation regime
18 : Due to sea level change
19 : Due to the precipitation/evaporation regime
20 : Due to sea level change
21 : Due to sea level change
22 : Due to Permafrost
23 : Due to soil development
24 : Due to Permafrost
25 : Due to soil development
26 : Due to soil development
27 : Due to Permafrost

**Figure B10. Tornado plot for the Sellafield-specific application of a branch of the System Properties ESL Model**

Comparison of the Tornado plots in Figures B9 and B10 illustrates a difference between the System Properties model and the EFEPs model. Inevitably, the more significant uncertainties in the interpretation of available evidence in terms of scenario development lie in making links between information on changes in system properties and the processes that were responsible for these changes. Hence the System Properties model shows greater explicit sensitivity to the evidence interpretation, whereas the EFEPs model captures these relationships only implicitly in the parameterisation of dependency.

### B5.3 Conclusions and recommendations about the utility of ESL

There were limitations to the time and resource available to carry out this trial application of the ESL method to an evaluation of palaeohydrogeological evidence. Therefore it is inappropriate to attempt to draw quantitative conclusions. It has already been stated that the ESL method was developed to ensure that all potentially relevant information is considered together within a common framework, thereby seeking to avoid the biases that may otherwise be introduced through inadvertent focus, or undue reliance, on particular 'favourite' sources or categories of evidence. It is therefore important that too narrow objectives or sub-sets of evidence are not used alone in a real demonstration of the ESL technique.

In practice, the ESL model of palaeohydrogeological evidence applied in this study inevitably invoked consideration of a wider range of types and sources of evidence than from the PADAMOT palaeohydrogeological project and, being focused on the implications for scenario selection for PA, it was recognised that some areas of the model cannot be addressed by palaeohydrogeological evidence alone. The complex decisions required rely on broad-ranging consideration and manipulation of a range of types and sources of evidence with relevant uncertainties.

It could be argued that the ESL approach is inappropriate for handling the geochemical and mineralogical data acquired in PADAMOT that depend so much on expert interpretation just to relate the data with the required information and judgments on sub-processes, let alone to the top-level process. However, after testing the ESL process, the PADAMOT participants judge that provided appropriate questions are asked and they can be legitimately addressed by the evidence, then there is merit in eliciting judgements concerning the quality and relevance of such evidence. This requires that the full potential evidence base is recognised and that an appropriate model structure is developed.

A difficulty with applying ESL to data derived in PADAMOT is the strong dependency between sub-processes that share common sources of information, because such information (e.g. evidence for salinity change) is not uniquely indicative of a particular process to the exclusion of others. The degree of dependency in these situations is not easy to assess. The use of alternative ESL models suggests how such uncertainties could in principle be addressed either through direct appraisal of the evidence itself in the System Properties model or through specification of the dependency parameter in the EFEPs model. It is clearly as important to understand the judgments that underpin decisions about model parameters as it is to document the process of evidence interpretation. This may make it desirable to apply the ESL approach so that the levels of dependency are as low as possible.

Scenario development for PA requires that all sources of evidence and judgement relating to the analysis of both past and potential future changes are deployed. ESL can help to ensure that assessment modellers, site investigators and geosphere/biosphere researchers, rather than being 'compartmentalised', work together within a single team with the common aim of challenging safety arguments and identifying, understanding and resolving uncertainties. Otherwise there are likely to be unresolved inconsistencies between interpreted palaeohydrogeological information and the scenarios adopted for performance assessment.

Although the ESL output is numeric, providing a quantified statement of support for or against a hypothesis (together with any residual uncertainty), it must be remembered that the process is based on subjective assignments of significance and quality. As such, the quantitative end results should not be implied to represent firm and unequivocal assessments concerning the support for a hypothesis or proposition. It would be especially dangerous to compare ESL results for alternative hypotheses that do not use the same underlying data (to state that one is better supported than the other for example).

It has to be admitted that the broad conclusion of this exercise is that the isolated use of palaeohydrogeological data and interpretations of the types that have been acquired in PADAMOT do not, in their current state of density and uncertainty, provide a strong basis for making unequivocal judgments on PA scenario-related decisions. This conclusion was already discussed in the brief review of palaeohydrogeology in PAs that was carried out at the start of PADAMOT by Bowden et al. (2002), and also appears to be the view of many people involved directly in PA work, as illustrated by the reviews in Section 2 of this report.

This exercise has identified that the rather broad interpretations of palaeohydrogeological data create large degrees of dependence among the child processes and large uncertainties that are propagated through the model to the parent process. This has resulted in a rather equivocal outcome with an evidence ratio close to one. To an extent, this outcome might be attributed to the top-level processes for the alternative formulations of the ESL model being null hypotheses, i.e. *'Establishing that climate-driven changes over the Quaternary have had little impact at repository depth'* or *'that System Properties have not been significantly modified by surface environmental change during the Quaternary'*. It is recognised that more substantiated statements to support these contentions might be forthcoming if a more rigorous exercise was to be undertaken and/or a wider knowledge base was used (e.g. evidence from natural analogues).

It must be stated that the process to develop an ESL model and parameterise it by eliciting measures of sufficiency, dependability and necessity is a time-consuming and potentially expensive endeavour. Furthermore, whilst application of the technique may identify areas for further targeted research and allow a structured consideration of the issues, the end result may sometimes have been intuitively obvious at the outset. Nevertheless, the value of ESL is to audit a documented process to justify such assumptions.

Despite the above concerns, the expert group considered their participation a valuable learning process, in terms both of general experience in the application of a systematic methods to evidence interpretation and of specific application to information derived from PADAMOT. The process that was followed in developing logical models to use palaeohydrogeological evidence in support of scenario development illustrates how this type of information could be framed to be usable by PA teams. The formalised approach engenders critical thinking about the way in which such evidence is assessed and interpreted. There can be little doubt that the rigourous process of testing the credibility of judgments and interpretations of relevant data for their use in constraining scenarios in PA is the most defensible approach. The ESL exercise reported here has catalysed critical thinking about palaeohydrogeological evidence. Equally, more consistent and thorough screening and development of assessment scenarios using all available evidence is required in PA.