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Features, Events and Processes Evaluation Catalogue for Argillaceous Media

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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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- to provide authoritative assessments and to forge common understandings on key issues, as input to government decisions on nuclear energy policy and to broader OECD policy analyses in areas such as energy and sustainable development.

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In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has a Co-operation Agreement, as well as with other international organisations in the nuclear field.

FOREWORD

Argillaceous media are being considered throughout the OECD/NEA member countries as potential host rocks for the final, safe, near-surface or at depth disposal of radioactive waste, and/or as a major constituent of the repository system in which waste will be emplaced. These media have indeed a number of favourable generic properties, e.g. homogeneity, low water flow, chemical buffering, propensity for plastic deformation and self-sealing of fractures, and marked capacity to chemically retard the migration of radionuclides.

For evaluating these geological media and notably for quantitatively assessing the potential migration of radionuclides to the environment, not only site-specific data from a site characterisation programme are required, but also a sound understanding of the basic physical and chemical processes that govern water, gas and solute transport through them. An important stage of the performance assessment is the identification and documentation of the features, events and processes that may be relevant to long-term safety.

In this context, the Working Group on the Characterisation, the Understanding and the Performance of Argillaceous Rocks as Repository Host Formations (known as "Clay Club") launched the FEPCAT (Features, Events and Processes CATalogue for argillaceous media) project in late 1998. The FEPCAT project aims at providing, for each FEP, a critical overview of conclusions and key references related to its current understanding and its potential impact on the long-term performance of the geosphere barrier, and information on ongoing and planned work. Experimental information (field, laboratory, numeric) provided by the funding organisations was the primary source of data.

Specifically, the main objectives were as follows:

- To derive a list of FEPs which are specific to argillaceous media. Only FEPs deemed relevant were to be included.
- To provide an overview of past, ongoing and planned *in situ* and laboratory experiments.
- To make a link between site investigations and their application in performance assessment, and to provide a scientific background for the assessment of geosphere performance.
- To define future priorities with regard to a better understanding of argillaceous media.
- To define terms whose connotation is different in different countries or scientific disciplines, and to link the radwaste terminology to general scientific usage.

The present document provides the results of work performed by an Expert Group to develop a FEPs database related to argillaceous formations, whether soft or indurated. It describes the methodology for the work performed, provides a list of relevant FEPs, summarises the knowledge on each of them, gives general conclusions and identifies priorities for future work.

A pdf version is available on the following website: http://www.nea.fr/html/rwm/clayclub.html.

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The national organisations represented within the Working Group on the Characterisation, the Understanding and the Performance of Argillaceous Rocks as Repository Host Formations (known as “Clay Club”) and the NEA wish to express their gratitude to the authors of this report: M. Mazurek (Switzerland), F. J. Pearson (USA), G. Volckaert (Belgium) and H. Bock (Germany).

This project was supported by a consortium of national organisations: Andra (France), Enresa (Spain), IRSN (France), JNC (Japan), Nagra (Switzerland), Nirex (United Kingdom), Ondraf/Niras and SCK•CEN (both Belgium). These organisations are thanked for their financial support and for their technical input.

The following external experts are also thanked for their contribution by filling in questionnaires for selected FEPs: J. Katsube (Canada), B. Krooss (Germany), C. Neuzil (USA), Puram and Mecsek Ore Environment (both Hungary). T. Sumerling (United Kingdom) is acknowledged for contributing to the structuring of the FEPs list.

Valuable technical and administrative support was provided by J. C. Mayor (Chairman of the FEPCAT Steering Group, Enresa), P. Lalieux (Clay Club Chairman, Ondraf/Niras), Marc Thury (past Clay Club Chairman, Nagra) and Sylvie Voinis (NEA secretariat). A review of a previous draft of this report was also provided by GRS (Germany).

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SECTION I

Framework and Lessons Learned

1. INTRODUCTION

The FEPCAT (**F**eatures, **E**vents and **P**rocesses **CAT**alogue for argillaceous media) project was launched by the OECD/NEA Clay Club in late 1998. This initiative was motivated by the growing international interest in argillaceous formations as hosts of geological repositories for radioactive waste. A number of sites are currently being investigated, and underground research laboratories are in operation. FEPCAT was funded by Andra (France), Enresa (Spain), IRSN (France), JNC (Japan), Nagra (Switzerland), Nirex (United Kingdom), Ondraf/Niras (Belgium) and SCK•CEN (Belgium). Each of these organisations nominated a delegate to the Steering Group, which was chaired by J.C. Mayor (Enresa). The technical work was carried out by the Expert Group, i.e. the authors of this report, under the co-ordination of Martin Mazurek. The project was subdivided into the following stages:

1. Definition of a list of FEPs (Features, Events, Processes) by the Expert Group. Design of a questionnaire prompting all participating organisations for technical input.
2. Provision of technical input in questionnaire format by all participating organisations.
3. Compilation and synthesis of the information by the Expert Group.

Further information for a small number of FEPs was provided by External experts, i.e. scientists with relevant knowledge of selected aspects of clay science. These included J. Katsube (Canada), B. Krooss (Germany), C. Neuzil (USA) and the Hungarian team of Mecsek Ore Environment and Puram.

The Expert Group consisted of the following members:

Name	Affiliation	Expertise
Helmut Bock	Q + S Consult, Bad Bentheim, Germany	Geomechanics. Mechanical interpretation of geological structures. *In situ* stress regimes and their measurement. Laboratory and field testing. Engineering of sub-surface structures and performance assessment.
Martin Mazurek	Rock-Water Interaction, Institute of Geological Sciences, University of Bern, Switzerland	Interactions between minerals, aqueous fluids and gases. Structural geology and relationship to hydrogeology. Impact of geologic system properties and processes on the performance/safety of the geologic barrier.

Name	Affiliation	Expertise
F. Joe Pearson	Ground-Water Geochemistry, New Bern, North Carolina, USA	Geo- and hydrochemistry, isotopic geo- and hydrology in various formations. Characterisation of mudrock porosities and of their relationship to pore-water chemistry and transport properties.
Geert Volckaert	Waste and Disposal Department, Nuclear Energy Research Centre, SCK•CEN, Mol, Belgium	Performance assessment. Gas migration and hydrogeology in soft and indurated argillaceous formations. Radionuclide transport in soft, plastic clays.

1.1 Objectives of the FEPCAT project

The FEPCAT project aims at providing each FEP with a critical overview of conclusions and key references related to its current understanding and its potential impact on the long-term performance of the geosphere barrier, and information on ongoing and planned work. Experimental information (field, laboratory, numeric) provided by the funding organisations is the primary source of data.

Specifically, the main objectives were as follows:

- To derive a list of FEPs which are specific to argillaceous media. Only FEPs deemed relevant were to be included.
- To provide an overview of past, ongoing and planned *in situ* and laboratory experiments.
- To make a link between site investigations and their application in performance assessment (PA), and to provide a scientific background for the assessment of geosphere performance.
- To define future priorities with regard to a better understanding of argillaceous media.
- To define terms whose connotation is different in different countries or scientific disciplines. Link the radwaste terminology to general scientific usage.

In order to meet these objectives, a substantial degree of generalisation of the information provided by the organisations is needed. The applicability of the results and conclusions of the FEPCAT project to specific sites and disposal projects would require another step in which the site- and project-specific features and boundary conditions are considered. For example, the PA relevance of a FEP depends on specific factors such as repository design, type of waste or regulatory demands.

In retrospect, the main technical challenges of the project included:

1) bridging the wide scientific spectrum (geology, geochemistry, hydrogeology, rock mechanics, engineering);
2) the integration of information from different sources (laboratory, underground research laboratory, borehole, field, natural analogue, numerical model, open scientific literature); and

3) the establishment of a link between data acquisition and process understanding on the one hand and the use of this information in performance assessment on the other hand.

The FEPCAT project does not claim to provide an exhaustive characterisation for each FEP, covering the complete spectrum of all scientific and PA-related aspects. By the nature of its structure and philosophy, it includes expert judgement to some degree and, for the application to a disposal project, requires the consideration of system-specific boundary conditions. The emphasis is on integration and knowledge management ("guide book"), not on the details of interest to specialists in very specific fields. FEPCAT has not been designed to provide a catalogue of quantitative values to be used directly as input to PA calculations.

1.2 Scope

The FEPCAT project:

- focuses on FEPs related to deep geological disposal and covers all types of argillaceous rocks, whether soft or indurated;
- is independent of the type of radioactive waste disposal planned (spent fuel, vitrified high-level waste, TRU waste, low-level waste);
- focuses on the geosphere (including the affected field and the excavation-disturbed zone, i.e. all effects related to the existence of the repository) but excludes the engineered barriers *per se*;
- considers only FEPs with post-closure effects over a time period in the order of 1 Ma;
- excludes waste retrieval and all human activities after the closure of the repository;
- focuses on a limited number of high-probability FEPs but disregards FEPs deemed less important or unlikely to occur. Technical detail is more important than completeness;
- focuses on FEPs that have specific characteristics in argillaceous rocks;
- considers each FEP in isolation (no scenario analysis);
- has no ambition to judge national programmes.

1.3 Closing dates

Most of the information that was provided by the participating organisations dates from the year 2000. The Expert Group included more recent information wherever it was easily available. However, no formal update could be performed, and the completeness of the most recent information cannot be guaranteed at this stage. Relevant reports that became available during the final stages of the FEPCAT project and thus were not considered in full include:

SAFIR-2 (Boom Clay, Belgium; Ondraf/Niras, 2002)

Référentiel géologique (Callovo-Oxfordian, France; Andra, 1999a)

Opalinus Clay synthesis (Switzerland; Nagra, 2002)

Geochemical synthesis of the Mont Terri Underground Laboratory (Opalinus Clay, Switzerland; Pearson *et al.*, 2003).

1.4 Definitions and abbreviations

Advection-dominated transport	In an argillaceous formation, advection may become the dominant transport process if preferential flow along fractures within the formation occurs over the spatial scales considered in PAs. This means that advection-dominated transport is important if a formation contains a connected fracture network and if the fractures have, at least episodically, a transmissivity well above that of the unfractured rock mass.
Diffusion-dominated transport	Diffusion is the dominant transport mechanism (over spatial scales considered in PAs) in argillaceous formations that are devoid of connected fracture networks and in fractured formations where fracture transmissivity is similar to that of the unfractured rock matrix (e.g. due to self-sealing processes).
EDZ	Excavation-disturbed zone. In this report, this term relates to the zone around underground openings where plastic (irreversible) and/or elastic (reversible) deformation took place in response to the excavation. Thus the term "EDZ" as used here does not refer exclusively to the zone where macroscopic fractures developed but to a larger region. There is no universally accepted definition, and the matter is discussed in NEA (2002b).
FEP	Feature, event or process potentially relevant for the evaluation of long-term safety of a geological waste repository (see also NEA, 2000).
Performance assessment (PA)	Analysis of the performance of the system concept, with the aim of developing confidence that the system will (or can be designed to) perform within acceptable bounds. May include, but is not limited to, a range of quantitative analyses of radionuclide release from, and migration through, individual system components.
Safety assessment	Process of evaluating long-term performance, compliance with acceptance guidelines and confidence in the safety indicated by the assessment results. Performance assessment is a necessary input to safety assessment.
Safety case	Collection of arguments, at a given stage of repository development, in support of the long-term safety of the repository. A safety case comprises the findings of a safety assessment and a statement of confidence in these findings. It should acknowledge the existence of any unresolved issues and provide guidance for work to resolve these issues in future development stages. A safety case is the end product of a safety assessment.

Clay, shale & lithologic terms

There is no generally accepted terminology of argillaceous sediments and sedimentary rocks (see also discussion in Horseman *et al.*, 1996, ch. 2.1). Existing classification schemes use grain size, degree of induration and texture (e.g. lamination, fissility) as criteria. However, they are not all consistent (compare e.g. Potter *et al.*, 1980 and Blatt *et al.*, 1980) and, more importantly, many of the terms coined in those classifications are not currently used (e.g. “claymud”, “mudshale”). Aplin *et al.* (1999) discuss these difficulties and propose to use the terms “mud” and “mudstone” in a broad sense, including all clastic sediments and sedimentary rocks where grain size is primarily <62.5 µm. The term “clay” refers to a non-indurated clastic sediment where >66% of the rock has a grain size below 4 µm, and “claystone” is the indurated analogon. “Shale” is not defined in a consistent way, but is sometimes used as a synonym of “argillaceous sediment and sedimentary rock”, and sometimes to describe an indurated argillaceous sedimentary rock only. There is a general agreement that “argillite” describes a highly indurated, low-grade metamorphic argillaceous rock.

In this report, the term “clay” will be used to address weakly consolidated lithologies rich in clay minerals, such as the Boom or Yper Clays in Belgium. In contrast, “shale” will be used to describe more strongly consolidated units, such as the Toarcian-Domerian at Tournemire (France). It also needs to be noted that, for historic reasons, formation names are not necessarily consistent with current lithological terminology, e.g. in the case of Opalinus Clay or the Boda Clay Formation (which will be addressed as shales in this report).

2. PRESENTATION OF SITES CONSIDERED IN THE PROJECT

2.1 Callovo-Oxfordian at Bure, France

In the eastern part of the Paris Basin, Andra is investigating a site near Bure (also called "Site Meuse-Haute Marne" or "Site de l'Est"), mainly targeting a flat-lying, *ca.* 130 m thick argillaceous formation of Callovo-Oxfordian age at 420-550 m below surface. Three deep boreholes were drilled and investigated. These investigations provided the basis for an extensive report (Référentiel géologique). Currently, shaft-sinking activities are underway for an underground research laboratory in the Callovo-Oxfordian formation. Should future investigations corroborate the suitability of the site, it is envisaged to build a repository for high-level waste.

Investigations performed mainly by: Andra, France. Key reference: Andra (1999a).

2.2 Toarcian-Domerian at Tournemire, France

In 1989-1990, IRSN initiated *in situ* research in argillaceous formations. An underground research laboratory was built in 2 galleries excavated from a former railway tunnel near Tournemire (Aveyron, southern France). The tunnel is 110 years old and 1885 m long. It penetrates a flat lying, 250 m thick Liassic argillaceous series (Domerian and Toarcian marls and shales).

The Tournemire project aims at generic studies related to the disposal of radioactive waste. The main geological, stratigraphic, tectonic and hydrogeological characteristics of the site are studied. The research programme deals mainly with the hydrogeological properties, in order to characterise fluid flow and solute transport through the argillaceous formation and to quantify the relevant processes in numeric models.

The site is not under consideration for a real radioactive waste repository, but provides support for generic studies for this purpose.

Investigations performed mainly by: IRSN, France. Key references: Boisson *et al.* (1998), Cabrera *et al.* (2001).

2.3 Spanish Reference Clay, Spain

The Spanish Reference Clay refers to one of the numerous argillaceous formations retained in Spain for future characterisation studies when so decided by the Spanish authorities.

Investigations performed mainly by: Enresa, Spain. Key reference: Enresa (1999).

2.4 Opalinus Clay at Mont Terri, Switzerland

The Mont Terri underground research laboratory is located in north-western Switzerland (Canton Jura) and consists of a tunnel parallel to a security tunnel and to the main tunnel of a motorway across the Mont Terri anticline in the Folded Jura Mountains. It is located in Opalinus Clay, a middle Jurassic marine shale formation. The formation is over-consolidated and *ca.* 270 m below surface at laboratory level. Research was started 1996 and will be documented in synthesis reports on geochemistry (available), hydrogeology and rock mechanics (in preparation). In future, the main focus will be long-term experiments.

Investigations performed mainly by: Mont Terri international consortium. Key references: Thury & Bossart (1999), Pearson *et al*. (2003).

2.5 Opalinus Clay in the Zürcher Weinland, Switzerland

In 1994, the Opalinus Clay (a Middle Jurassic marine shale formation) was identified as the priority sedimentary host rock option for the disposal of spent fuel and vitrified high-level waste in Switzerland, and the Zürcher Weinland (north-east Switzerland) as the first-priority area for site-related investigations. Detailed characterisation of the host rock and the potential siting area followed after 1994. The key elements of this research programme were a 3-D seismic campaign in the Zürcher Weinland covering an area of around 50 km^2, an exploratory borehole (Benken), experiments as part of the international research programme in the Mont Terri underground research laboratory (Canton Jura), comparative regional studies on the Opalinus Clay including deep boreholes in the near and far vicinity of the siting area, and comparisons with clay formations that are under investigation in other countries in connection with geological disposal.

Investigations performed mainly by: Nagra. Key reference: Nagra (2002).

2.6 Boom Clay at Mol, Belgium

The Boom Clay under the nuclear site of Mol/Dessel in the north-east of Belgium is considered as the Belgian reference host formation for the methodological study of the disposal of long lived medium and high level radioactive waste in deep clay layers. The first characterisation works under the site were launched in 1975 by the Nuclear Energy Research Centre of Mol (SCK•CEN). Since that time three sampled deep drillings with extensive geophysical logging and two high resolution seismic campaigns have been carried out on site, moreover, a large number of parameters of different natures have been determined in laboratory and/or *in situ*. An underground research laboratory at the depth of 220 m (HADES-URF) was built and progressively extended for numerous *in situ* experiments. In the framework of the PRACLAY project (a large-scale demonstration test) the HADES-URF has recently been extended. A second shaft and a connection gallery have been built.

Investigations performed mainly by: Ondraf/Niras and SCK•CEN, Belgium. Key reference: Ondraf/Niras (2002).

2.7 Ypresian Clays at Doel, Belgium

Ypresian Clays (Kortrijk and Tielt Formations) under the Nuclear Site of Doel along the River Schelde in North Belgium are considered, on governmental request, as alternative host rocks to the Boom Clay for the methodological study of the disposal of long lived medium and high level radioactive waste in deep clay layers. The characterisation works under the site were launched in 1995 by the drilling of fully cored deep boreholes with extensive geophysical logging. No underground research laboratory exists at Doel.

Investigations performed mainly by: Ondraf/Niras and SCK•CEN, Belgium. Key reference: Ondraf/Niras (2002).

2.8 Boda Clay Formation, Hungary

The Boda Clay Formation occurs in SW Hungary, W of the city of Pécs. The Permian, 250-260 Ma old formation is known to occur over an area larger than 150 km^2. A comprehensive characterisation programme was carried out here between 1993 and 1999. An underground research laboratory was run at a depth of 1 030-1 080 m below surface in a tunnel excavated from an existing tunnel previously built for mining purposes. Work was discontinued after 1999, and the tunnel system has been flooded.

The formation originates from lacustrine sediments deposited under oxidising and alkaline conditions. The main lithology are albitic claystones. The formation was buried to 3.5-4.5 km below surface and so is highly indurated. It contains fractures and faults originating from a number of tectonic events. Solute transport is dominated by advection in brittle structures.

Investigations performed mainly by: Mecsek Ore Environment and Puram, Hungary. Key references: Kovacs (1999, 2003).

2.9 Mizunami Group at Tono, Japan

The Miocene sedimentary cover of the basement (mostly Cretaceous granitic rocks) of the Tono region has been investigated in connection with the uranium exploration activities and palaeontological and geoscientific studies. It is being characterised in the course of the drilling and mining activities for the planned underground research laboratory (in granitic basement) at the nearby locality of Mizunami. The thickness of the sedimentary cover is variable, between 0 and several hundreds of metres.

Miocene argillaceous sequences include the Toki Lignite-bearing Formation (non-marine; basal conglomerate, sandstone and mudstone interbedded with lignite-bearing facies, hosting uranium ore bodies; up to 170 m in thickness), the Akeyo Formation (marine; mudstone and tuffaceous sandstone interbedded with pumice tuff; up to 280 m in thickness) and the Oidawara Formation (marine; basal conglomerate and massive siltstone and mudstone; up to 160 m in thickness). These sedimentary sequences are cut by the Tsukiyoshi fault with vertical reverse displacement about 30 m in the Tono mine.

Investigations performed mainly by: JNC and Mizunami Fossil Museum, Japan. Key reference: Yusa *et al.* (1993).

2.10 Palfris Formation at Wellenberg, Switzerland

In 1993, following a comprehensive investigation programme including 7 exploratory boreholes, a site at Wellenberg was selected for the disposal of low and intermediate level waste. Wellenberg is located in Central Switzerland (Canton Nidwalden) in the Helvetic Alps, which lie along the northern margin of the Alps. The investigated potential host rock consists of the very low permeability Palfris Formation (dominating by volume, mainly argillaceous marls) and the Vitznau Marls of the Drusberg nappe, including Interhelvetic Mélange and Tertiary shales of the Axen nappe. The Palfris Formation is one of the major décollement horizons of the Helvetic Alps and, although normally only 200 m thick, at Wellenberg has been thickened by tectonic processes (folding, imbrication) to a large mass exceeding 1000 m. All these rocks were buried to *ca.* 10 km below surface some 20 Ma ago and so are highly indurated.

For any underground construction and investigation, a Cantonal mining license is required in addition to Federal permits. This gives the Canton the right to veto a project, even when already licensed by the Federal Government. In Nidwalden, this Cantonal license is subject to popular referendum. In 2002, an application for a concession for an exploratory drift to allow further geological investigation of the site was rejected by the people of Nidwalden and therefore the site was abandoned from further consideration.

Investigations performed mainly by: Nagra, Switzerland. Key reference: Nagra (1997).

2.11 Pierre Shale in south Dakota, USA

The Pierre Shale is a Cretaceous, smectite-rich unit occurring in large parts of the western USA and Canada, with thickness between 0 and *ca.* 2 000 m and a high porosity of *ca.* 30 vol%. Most of the relevant work was done in central south Dakota (Pierre Shale cropping out on the surface).

Investigations performed mainly by: US Geological Survey. Key references: Neuzil (1993, 1995a).

2.12 Couche silteuse at Marcoule, France

The flat-lying Couche silteuse at Marcoule (Gard, southern France) is a Cretaceous silty to argillaceous formation (*ca.* 200-400 m thick) that has been investigated since 1994 as a potential site for an underground research laboratory and repository in France. After the decision to focus activities on the Callovo-Oxfordian at Bure, the investigations were discontinued. Most available information is based on 3 deep boreholes.

Investigations performed mainly by: Andra, France. Key reference: Andra (1999c).

3. DERIVATION AND PRESENTATION OF THE FEPS LIST

3.1 BOGSAT approach

In a first stage, FEPs were collected on the basis of several national FEPs lists (Ondraf/Niras & SCK•CEN: Marivoet 1994, Bronders *et al.* 1994; Enresa: Enresa 1998a,b; Nagra: Gribi *et al.*, 1998, Sumerling 1998), and by personal contributions of a number of experts. This approach to data collection ("Take whatever is available and compile in useful format") is inherently unstructured and therefore called the "BOGSAT" (Bunch Of Guys Sitting Around a Table) approach (see Figure 1). While the resulting FEPs list is clearly linked to existing data, it depends, to some degree, on the maturity of the projects, on the preferences and biases of the underlying documents and opinions and so does not provide a way to check completeness. The FEPs list derived by this approach contained 526 FEPs. At this stage, the list had no hierarchical structure or logical order and contained numerous redundancies, often explicit repetitions. A first FEPs screening was undertaken, applying the following exclusion criteria:

- FEPs beyond the scope of FEPCAT as defined in Section I, Chapter 1.2 (e.g. retrievability, human activities);
- FEPs beyond timeframe of FEPCAT (order of 1 Ma);
- FEPs too general or too detailed and/or already covered by other FEPs (repetitions and evident redundancies);
- FEPs not specific to argillaceous media (e.g. meteorite impact);
- FEPs related exclusively to underground repository elements (e.g. waste, engineered barrier system);
- FEPs irrelevant for current repository designs (e.g. co-disposal with other hazardous wastes);
- FEPs of secondary priority (according to the judgement of the Expert Group; e.g. effects of radiation on geosphere materials).

This first stage of screening resulted in a reduction of the number of FEPs to 290.

Figure 1. **Approaches for the derivation of FEPs lists**

BOGSAT approach	Top-down approach
B unch **O** f **G** uys **S** itting **A** round a **T** able	*Key question: What is the radionuclide release at the downstream boundary of the clay body as a function of time, and how can we quantify it ?* A. Undisturbed system properties ("far field") *Advection/dispersion* *Coupled transport* *Retardation* B. Repository-induced perturbations (EDZ, "affected field") *Advection/dispersion* *Coupled transport* *Retardation* C. External perturbations (geologic, climatic, human) *Advection/dispersion* *Coupled transport* *Retardation*

In a second stage, the remaining 290 FEPs were thematically grouped according to the following topics (in alphabetic order):

chemical reaction
clay min.-porewater interaction
colloids
deformation events
diagenesis
diffusion
dilution
EDZ diverse
flow
flow, two-phase
gas from repository
gas, natural
geomechanics
high pH
human
hydrochemistry
lithology
matrix porosity
microbial
migration pathways
mineralogy
organics, from waste
organics, natural
osmosis
oxidation
saturation
solubility
sorption (broad definition)
stress field
swelling and self-healing
thermal
thermal, desiccation
uplift, subsidence, erosion

The list of topics above has been compiled on the basis of the existing FEPs list, i.e. it is not an independent check of completeness based on a structured approach. A second FEPs screening stage was so performed according to the following criteria:

- Further elimination of redundancies and partial overlaps among FEPs.
- Achievement of a consistent degree of detail, i.e. elimination of very detailed FEPs. For example, a FEP “Fracture aperture changes in consequence of interaction between hyperalkaline water and clay minerals” would be eliminated because it is covered by “Hyperalkaline plume”.

The reduction of the number of FEPs from this screening was substantial, ending up with 93 FEPs.

3.2 Top-down approach

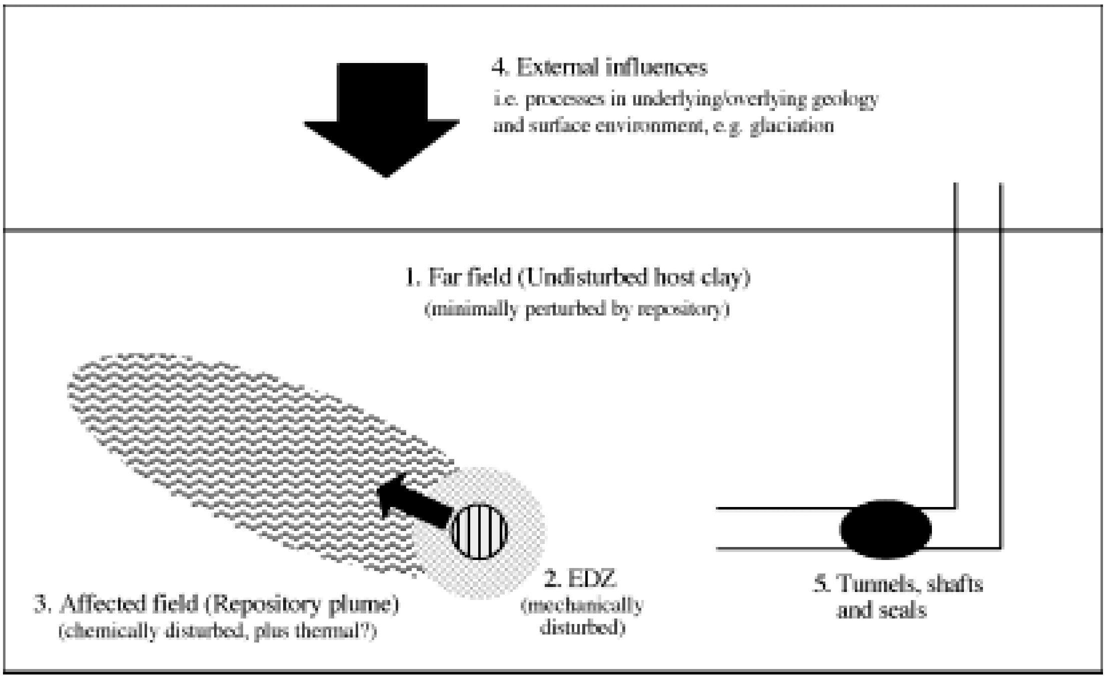
While the size of the FEPs list was now manageable, it had no obvious hierarchy and no clear link to transport modelling or PA. Thus it is not straight-forward how its completeness can be checked, and how it can be made useful for performance assessment issues. At this stage, it was necessary to incorporate the modelling perspective explicitly into the FEPs selection methodology.

A repository environment consists of a number of system components, i.e. spatial units with different characteristics, as shown in Table 1 and Figure 2.

Table 1. **System components of a deep geological repository**

System component	Definition / Explanations
Repository elements	Comprises waste and engineered barriers
Excavation-disturbed zone (EDZ)	Zone where the host rock is mechanically affected by tunnel excavation.
Affected field	Zone in host rock beyond the EDZ that is affected by the presence of the repository (e.g. chemical and hydraulic effects).
Far field	Zone in host rock unaffected by the presence of the repository (“natural” system) with the exception of some transient effects (e.g. thermal pulse from high-level radioactive waste, pore-pressure drawdown around tunnels).
External influences	Describes processes originating outside the host rock and includes the geological long-term evolution, climatic and human effects
Tunnels, shafts and seals	Describes the access openings to the repository.

Figure 2. **System components of a repository environment**



Repository elements, tunnels, shafts and seals *per se* are beyond the scope of FEPCAT. The same is true for external influences based on human action (see Section I, Chapter 1.2).

A disposal system hosted by an argillaceous formation will generally be arranged so that some sensible thickness of the formation is *not* substantially disturbed by the presence of the repository, so that the excellent properties of undisturbed rock can be invoked in the safety case. Indeed, there is a large experimental body aimed at investigating radionuclide migration where every effort has been made to minimise perturbations. In addition, the usual scientific method is to understand a system in its simplest (undisturbed?) state, and then to understand the effect of perturbations. In a repository system, perturbations are related to the existence of the repository or due to external effects (see Figure 1 and 2). Thus, from a modelling perspective, the first-order structuring of FEPs distinguishes

A. The undisturbed system (or, the “far field”): Transport occurs by a number of possible *transport mechanisms*, and it is counteracted by a number of *retardation mechanisms*. Models that quantify transport and retardation can be checked for consistency with independent information (e.g. ground-water residence times), and it is here where “soft” data come into play. Thus for modelling radionuclide migration through the undisturbed system, a FEPs list could be structured as follows:

A1 Transport mechanisms

A2 Retardation mechanisms

A3 System understanding and independent methods/tools to build confidence in predictive models

B. Repository-induced perturbations (including the excavation-disturbed zone (EDZ) and the “affected field”): These perturbations can be subdivided according to the different driving forces of the perturbations:

B1 Chemical perturbations
B2 Thermal perturbations
B3 Geomechanical perturbations
B4 Hydraulic perturbations
B5 Perturbations from coupled processes
B6 Perturbations from waste-derived gas
B7 Microbiological perturbations

C. External perturbations (geological long-term evolution in a broad sense): It is not straightforward to include external effects on the argillaceous formation into a top-down approach. Long-term effects can affect both transport and retardation mechanisms, with numerous and complex interdependencies. Thus many of the external effects are not directly integrated in transport models, and their effects are studied by separate sub-models or in more qualitative terms. Structuring the external effects was done according to the possible groups of phenomena:

C1 Diagenesis
C2 Deformation events
C3 Erosion and burial.

3.3 The structured FEPs list

The top-down approach discussed in the last chapter resulted in a structured FEPs framework which was derived independently, i.e. without the use of pre-existing FEPs databases from the literature. In the next step, the 93 FEPs from the BOGSAT approach were screened through this approach, with the following results:

- The integration was successful in that all 93 FEPs from the BOGSAT list could easily be allocated to a logical position in the structured list. This indicates that the suggested way of structuring is practicable.

- In the integration procedure, FEPs from the BOGSAT list were allocated to different hierarchical levels – e.g. “diagenesis” would be a higher hierarchy, whereas “Evolution of pore fluid” is one of many effects of diagenesis and so is placed at lower hierarchical levels. The development of structured FEPs lists more clearly shows the interrelations of FEPs than flat lists. Moreover, in a structured list it is possible to cut off the degree of detail to which FEPs should be explored as a function of resources or state of knowledge in a particular field. For example, a FEP entitled “Coupled processes due to repository-induced perturbations” can be split up into sets of more detailed FEPs that describe the individual couplings, e.g. thermo-mechanical, thermo-chemical, etc.

- A limited number of new FEPs emerged from the structured FEPs list that has not been represented in the FEPs list derived from the BOGSAT approach. This indicates that, with some exceptions, the latter information is largely comprehensive.

The resulting structured FEPs list contained 74 unique entries and was used as the basis for the questionnaires that were distributed to all participating organisations.

During the compilation of the answers to the questionnaires by the Expert Group, further simplifications became necessary:

- The FEP “Dilution” turned out not to have any characteristics specific to argillaceous formations and was deleted.

- Substantial answers for a number of FEPs were very limited (no answers came in at all for some FEPs). This was due to a too high degree of detail and/or the limited PA relevance of these FEPs according to the judgement of the national organisations. However, the lack of information in itself was not a criterion for removing FEPs. Such FEPs remained in the list but were merged with others, which resulted in a reduction to 59 FEPs. FEPs groups where the number of answers was limited include:

  B1 Chemical perturbations

  B5 Perturbations from coupled processes

  B6 Perturbations from waste-derived gas

  B7 Microbiological perturbations.

  C2 Deformation events

  C3 Erosion and burial.

Thus major changes were performed in section C of the FEPs list (long-term evolution), some changes in section B (repository-induced perturbations), while section A (undisturbed system) remained almost unchanged.

The final version of the structured FEPs list with 59 entries is presented in Table 2. It contains some features that need expanding further:

- The first column represents the running number of each FEP. This number is the basis for the structuring of Section II of this report.

- The second column represents the hierarchical number of each FEP.

- Some of the higher-hierarchy FEPs are fully covered by FEPs in lower hierarchies, i.e. they are general titles to a group of FEPs that need not to be considered (e.g. “Sorption”). Therefore, such FEPs do not have a running number.

- The structured FEPs list in Table 2 contains redundancies. For example, “diffusion” is a transport process in argillaceous media in which advection is not relevant. In fractured, indurated shales, advection may be the dominant transport process, and “matrix diffusion” is a retardation mechanism. Whether diffusion is considered to be a transport or a retardation mechanism, the same underlying process and set of parameters can describe it. Another example is “Self-sealing”, a process that plays a role both in the EDZ (i.e. in section B, repository-induced perturbations) and in natural fractures (i.e. in section C, long-term evolution). Such intentional duplicate entries are indicated in column “Related FEPs” of Table 2. Duplicate FEPs have identical running numbers.

Table 2. **Structured FEPs list**

FEPs no. and hierarchy		Structured FEPs classification	Related FEPs
	A	UNDISTURBED SYSTEM	
	A1	**Transport mechanisms**	
1	A1.1	Advection/dispersion	
2	A1.1.1	*Size and geometry of the host rock and of surrounding units, migration path length*	
3	A1.1.2	*Migration pathways, including heterogeneity and anatomy*	
4	A1.1.3	*Undetected geological features*	
5	A1.1.4	*Hydraulic potentials and gradients in the host rock, including boundary conditions*	
6	A1.1.5	*Hydraulic properties of the host rock*	
7	A1.1.6	*Units over- and underlying the host formation: local and regional hydrogeologic framework*	
	A1.2	Diffusion	A2.1
8	A1.2.1	*Diffusivity*	A2.1.1
9	A1.2.2	*Connected matrix porosity*	A2.1.2
10	A1.2.3	*Ion exclusion*	A2.1.4
11	A1.2.4	*Surface diffusion*	A2.1.5
12	A1.3	Colloid formation, transport and filtration	
	A2	**Retardation mechanisms**	
	A2.1	Matrix diffusion	A1.2
8	A2.1.1	*Diffusivity*	A1.2.1
9	A2.1.2	*Connected matrix porosity*	A1.2.2
13	A2.1.3	*Flow-wetted surface and accessibility of matrix*	
10	A2.1.4	*Ion exclusion*	A1.2.3
11	A2.1.5	*Surface diffusion*	A1.2.4

FEPs no. and hierarchy		Structured FEPs classification	Related FEPs
	A2.2	Sorption (broad definition)	
14	A2.2.1	*Lithology, mineralogy of rocks and fracture infills*	
15	A2.2.2	*Natural organics, complexation*	
16	A2.2.3	*Mineral-surface area*	
17	A2.2.4	*Pore- and fracture water composition*	
18	A2.2.5	*Dissolution / precipitation of solid phases*	
19	A2.2.6	*Solid solutions / co-precipitation*	
20	A2.2.7	*Ion exchange*	
21	A2.2.8	*Surface complexation*	
22	A2.2.9	*Thermodynamic and kinetic modelling data*	
	A3	**System understanding and independent methods / tools to build confidence in predictive models**	
23	A3.1	Palaeo-hydrogeology of the host formation and of embedding units	C1.1.1
24	A3.2	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units	C1.1.2
25	A3.3	Water residence times in the host formation	
	B	REPOSITORY-INDUCED PERTURBATIONS	
	B1	**Chemical perturbations**	
26	B1.1	Oxidation of the host rock	
27	B1.1.1	*Redox buffering capacity of the host rock*	
28	B1.2	Effects of repository components on pore-water chemistry in the host rock	
29	B1.2.1	*Interactions of hyperalkaline fluids and host rock*	
30	B1.2.2	*Organics from waste and their effect on transport properties of the host rock*	
	B2	**Thermal perturbations**	
31	B2.1	Thermal effects on mineral stability and pore-water composition	
32	B2.2	Thermal rock properties	
33	B2.3	Thermally induced consolidation of the host rock	
	B3	**Geomechanical perturbations**	
34	B3.1	Geomechanical stability	
35	B3.2	Size and structure of the EDZ	
36	B3.3	Effects of bentonite swelling on the host rock	
37	B3.4	Geomechanical rock properties	

FEPs no. and hierarchy		Structured FEPs classification	Related FEPs
	B4	**Hydraulic perturbations**	
38	B4.1	Hydraulic properties of the EDZ	
39	B4.2	State of saturation of the EDZ and desiccation cracking	
	B5	**Perturbations from coupled processes**	
40	B5.1	Coupled thermo-hydro-mechanic processes	
41	B5.2	Swelling	C2.3
42	B5.3	Self-sealing	C2.4
43	B5.4	Off-diagonal Onsager processes except chemical osmosis	
44	B5.5	Chemical osmosis	
	B6	**Perturbations from waste-derived gas**	
45	B6.1	Gas dissolution and chemical interactions between gas and pore-water	
46	B6.2	Gas migration through the primary porosity (matrix, natural fractures)	
47	B6.3	Gas migration through stress-induced porosity (gas fracs, pathway dilation)	
48	B6.4	Gas-induced transport in water	
49	B7	**Microbiological perturbations**	
	C	LONG-TERM EVOLUTION	
	C1	**Diagenesis**	
	C1.1	Past basin evolution	
23	C1.1.1	*Palaeo-hydrogeology of the host formation and of the embedding units*	A3.1
24	C1.1.2	*Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units*	A3.2
50	C1.1.3	*Past burial history*	
	C1.2	Ongoing and future processes	
51	C1.2.1	*Present and future geothermal regime and related processes*	
52	C1.2.2	*Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)*	

FEPs no. & hierarchy		Structured FEPs classification	Related FEPs
	C2	**Deformation events**	
53	C2.1	Past deformation events	
54	C2.2	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events	
41	C2.3	Swelling	B5.2
42	C2.4	Self-sealing	B5.3
55	C2.5	Present-day stress regime	
56	C2.6	Future stress regime	
	C3	**Erosion and burial**	
57	C3.1	Geomechanical effects of erosion / unloading	
58	C3.2	Consolidation due to burial	
59	C3.3	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)	

4. QUESTIONNAIRE STRUCTURE

A dedicated database and an electronic questionnaire form were developed in FileMaker (version 3.0) and sent out to all participating organisations and external experts with the following structure:

Q1 FEP name
Q2 FEP definition
Q3 FEP classification
Q4 Occurrence of FEP in different argillaceous media
Q5 Site-specific experimental information on FEP
  - *From in situ experiments*
  - *From a wider perspective of field information (e.g. natural analogues, palaeo-hydrogeology)*
  - *From laboratory experiments*
  - *From numerical experiments*
  - *Scaling issues and tools for up- and downscaling*

Q6 Level of understanding of FEP
  - *From a scientific perspective*
  - *From a performance assessment perspective*

Q7 Practical treatment of FEP in performance assessment
Q8 Coupling with other FEPs
Q9 Availability of synthesis or state-of-the-art reviews
  - *Site-specific*
  - *More general but radwaste-related*
  - *Open literature*

Q10 Planned work related to the FEP
  - *Field*
  - *Laboratory*
  - *Modelling*

Q11 Overall evaluation of FEP
Q12 Remarks
Q13 References

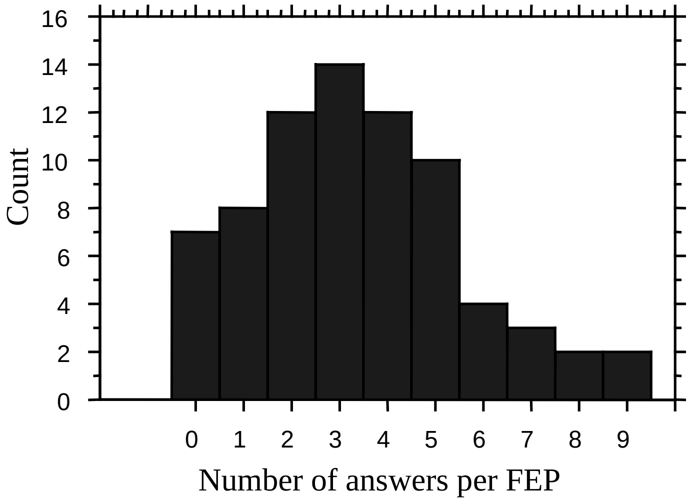
5. QUALITY AND NUMBER OF ANSWERS TO THE QUESTIONNAIRE

The national organisations participating in the FEPCAT project provided 179 answers to individual questionnaire forms. Approximately half of these were to-the-point, technically complete and therefore highly useful for the compilation work by the Expert Group. On average, this equals 2.4 answers, or 1.2 useful answers, per FEP. An additional 13 answers came from the Mont Terri Project. External Experts provided further 80 answers, of which 45 came from Mecsek/Puram (Hungary).

Figure 3 shows the distribution of the total number of answers per FEP. For the majority, 2-5 answers were received. For 15 FEPs, only one answer, or no answer at all, was received. The limited number of answers received for each FEP results from the following facts:

- Some of the participating organisations currently do not carry out work on a specific site in argillaceous rocks and therefore do not have complete data needed for filling in all questionnaire forms. Some others have experience from underground research laboratories, where only a limited number of FEPs were studied. Out of the participating organisations, only a minority have a recent and complete safety case.
- Answering the questionnaires was technically demanding work, as both field-related and PA-relevant aspects of each FEP had to be brought together. Within many organisations, only a very limited number of experts exist with the necessary technical background, and these are not fully available for projects such as FEPCAT. In retrospect, the questionnaire size and structure appears too ambitious.
- Some organisations that were heavily involved in national programmes did not have the manpower resources to convey all available information.

Figure 3. **Number of answers per FEP received by the Expert Group. About half of the answers were useful for the compilation work. (NB: The figure refers to the original FEPs list consisting of 74 entries)**



The Expert Group took the following measures to obtain as much information as possible:

- Workshops to kick off the questionnaire work were held at some organisations.
- Personal interviews were held with delegations of a number of organisations.
- A literature/report survey was done, mainly based on published and unpublished documents provided by the involved organisations, in some cases also draft versions.
- All organisations were asked to document why they did not provide any information on some FEPs ("blank FEPs"; see below).

6. DOCUMENTATION OF UNANSWERED FEPS (“BLANK” FEPS)

During the project, it was felt important to better justify the rationale behind unanswered FEPs. Therefore, each participating organisation that left a substantial number of FEPs unanswered was asked at a later stage about the reasons. The possible alternatives are given in Table 3, together with the summary of the answers obtained. Alternatives 1, 2 and 3 (29 answers) mean that there is no need to further pursue the FEPs. Alternatives 4 and 5 (129 answers) relate to FEPs that are regarded as potentially important, with a poor level of available information, so further actions or thoughts should be needed to improve their understanding. The relevance of alternatives 6 and 7 (52 answers) cannot be judged at the present stage.

Table 3. **Documentation of FEPs left blank in the questionnaires**

Alternative	**Number of answers**	
1. FEP is of limited relevance or totally irrelevant in our safety strategy/repository design.	26	29
2. FEP is potentially important, but we have no site-specific data. There is sufficient evidence from other sites or from the scientific literature that can be transferred to our site.	0	
3. FEP is potentially important, but we have no site-specific data. The FEP is difficult to investigate/quantify, so we cover it by conservative assumptions and/or sensitivity analysis.	3	
4. FEP is potentially important, but we have no site-specific data. We have not investigated the FEP due to other priorities or limitations in our programme.	121	129
5. We never thought of this FEP and so do not have any opinion.	8	
6. We have information on this FEP but did not fill in the questionnaire due to time constraints.	26	52
7. Other.	26	

The alternatives 4 and 5 are obviously of the most interest, i.e. FEPs that are considered as potentially relevant in PA with limited information. Table 4 indicates those FEPs that received 3 or more category 4 and 5 responses. Table 5 indicates those FEPs that received 2 answers.

Table 4 and Table 5 must be interpreted carefully. When a participating organisation did not have any data on a FEP, it was also unable to judge its potential relevance in PA. In such cases, it would typically choose alternatives 4 and 5. At the same time, other organisations may have investigated the FEP and concluded that it is not relevant.

This explains the discrepancies between Tables 4-5 and Table 7 below – in the latter Table, FEPs are classified on the basis of the compilation (Section II), i.e. based on the answers from organisations who *do have* relevant information. Therefore, Table 7 should be given more weight than Tables 4-5.

Table 4. **Documentation of FEPs left blank: FEPs with 3 or more answers stating that the FEP may be important, while information on the FEP is limited (alternatives 4 and 5 according to Table 3)**

FEP no.	**FEP name**
16	Mineral-surface area
28	Effects of repository components on pore-water chemistry in the host rock
33	Thermally induced consolidation of the host rock
43	Off-diagonal Onsager processes except chemical osmosis
44	Chemical osmosis
45	Gas dissolution and chemical interactions between gas and pore-water
46	Gas migration through the primary porosity (matrix, natural fractures)
47	Gas migration through stress-induced porosity (gas fracs, pathway dilation)
52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)
55	Present-day stress regime
56	Future stress regime
59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)

Table 5. **Documentation of FEPs left blank: FEPs with 2 answers stating that the FEP may be important, while information on the FEP is limited (alternatives 4 and 5 according to Table 3)**

FEP no.	FEP name
10	Ion exclusion
11	Surface diffusion
12	Colloid formation, transport and filtration
13	Flow-wetted surface and accessibility of matrix
23	Palaeo-hydrogeology of the host formation and of embedding units
24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
25	Water residence times in the host formation
30	Organics from waste and their effect on transport properties of the host rock
41	Swelling
42	Self-sealing
48	Gas-induced transport in water
49	Microbiological perturbations
51	Present and future geothermal regime and related processes
54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events
57	Geomechanical effects of erosion / unloading
58	Consolidation due to burial

7. INSIGHTS BASED ON THE COMPILATION

A number of issues common to many programmes and thus of wider interest emerged from the compilation of answers (Section II of this report). Some of these issues could be further addressed in the future on an international level.

7.1 Scaling issues

For a substantial number of FEPs, process understanding and parameter values are available based on observations and measurements in deep boreholes, in underground research laboratories and in laboratory experiments. However, uncertainties are related to the upscaling in space and time: PA-relevant spatial scales (*ca.* 100 m) are 2-4 orders of magnitude larger that those typically addressed by experiments (cm – m). Upscaling in time is also important; typical PA time scales in the order of *ca.* 1 Ma are 6-9 orders of magnitude longer than experimental time scales (typically 1 day to 1 year). According to the analysis of the FEPs compilation (Section II), temporal and spatial upscaling is considered as a major issue for the following FEPs:

FEP 1	Advection/dispersion
FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 4	Undetected geological features
FEP 6	Hydraulic properties of the host rock
FEP 8	Diffusivity
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 35	Size and structure of the EDZ
FEP 36	Effects of bentonite swelling on the host rock
FEP 37	Geomechanical rock properties
FEP 38	Hydraulic properties of the EDZ
FEP 41	Swelling
FEP 42	Self-sealing
FEP 46	Gas migration through the primary porosity (matrix, natural fractures)
FEP 47	Gas migration through stress-induced porosity (gas fracs, pathway dilation)
FEP 48	Gas-induced transport in water
FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)

FEP 54 Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

FEP 59 Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)

One powerful method to address upscaling issues is the use of information on the argillaceous formations as their own natural analogues. A number of features and parameters that can be measured or derived by indirect methods characterise the large-scale, long-term evolution of the host formation. These include interactions with its embedding units and, in some cases, integrate the long-term effects of episodic events (such as earthquakes) that may or may not have affected the host formation. As an example: in spite of substantial process understanding of self-sealing (FEP 42), geological evidence indicating the absence of rock/water interaction in faults (no fracture infills or alterations) remains among the best arguments that self-sealing of the formation operates over large scales in space and time. A full list of FEPs that are useful for upscaling other FEPs is given in Table 6.

Table 6. **List of FEPs that are useful for upscaling other FEPs in argillaceous rocks**

FEPs useful for upscaling issues		**FEPs that can be upscaled**	
FEP 5	Hydraulic potentials and gradients in the host rock, including boundary conditions	FEP 1	Advection/dispersion
		FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units	FEP 4	Undetected geological features
		FEP 6	Hydraulic properties of the host rock
		FEP 42	Self-sealing
		FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events
		FEP 59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units	FEP 1	Advection/dispersion
		FEP 8	Diffusivity
		FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)
FEP 25	Water residence times in the host formation		
FEP 50	Past burial history	FEP 6	Hydraulic properties of the host rock
		FEP 14	Lithology, mineralogy of rocks and fracture infills
		FEP 59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)

FEPs useful for upscaling issues		FEPs that can be upscaled	
FEP 51	Present and future geothermal regime and related processes	FEP 1	Advection/dispersion
		FEP 3	Migration pathways, including heterogeneity and anatomy
		FEP 4	Undetected geological features
FEP 53	Past deformation events	FEP 3	Migration pathways, including heterogeneity and anatomy
		FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

7.2 Demonstration of low permeability and limited relevance of advection

The demonstration of low permeability and the limited relevance of advection (FEP 1) are among the key objectives in many PAs for argillaceous host formations. Upscaling of laboratory data to the scale of the whole host formation is an important issue (see also Table 6). Relevant information referring to large scales in space and time can be derived from the following system characteristics:

1. Abnormal pressures in argillaceous formations.
2. Natural tracer profiles across argillaceous formations.

7.2.1 Normal and abnormal hydraulic pressures

Abnormal pressures (FEP 5) are usually interpreted as large-scale and long-term indicators of very low hydraulic conductivity and therefore are considered as an important input in any safety case. Even though very difficult to measure, they were observed at several sites (e.g. Callovo-Oxfordian at Bure, Opalinus Clay at Benken, Palfris Formation at Wellenberg, Pierre Shale in south Dakota). However, the underlying mechanisms explaining the abnormal pressures are not so well understood and different explanations exist for different sites. The use of abnormal pressures as indicators of maintenance of a non-equilibrium condition due to low permeability could be made stronger by addressing the following points:

- Identification of a small number of underlying mechanisms that explain abnormal pressures at all sites studied.
- Quantitative evaluation of these mechanisms at all sites as a consistency check. A mechanism that explains abnormal pressures at one site must equally well explain the observed absence of abnormal pressures at another site. For example, if chemical osmosis is thought to explain abnormal pressures at one site (e.g. Bure) and compaction due to burial to explain them at another site (e.g. Benken), then chamical osmosis at Benken and compaction at Bure need to be shown to be irrelevant.

These issues are well suited to be addressed in the framework of a co-ordinated international study. Potential benefits of such an effort include:

- A better understanding of the underlying processes and mechanisms leading to abnormal pressures.
- An improved basis for site-specific argumentation with respect to the large-scale and long-term hydrogeological evolution of the formation.

The first step in such a study would be the identification of gaps in the site-specific parameter sets and as far as reasonably possible the acquisition of missing data (e.g. pressure profiles or osmotic efficiencies).

7.2.2 Natural tracer profiles across argillaceous formations

A large number of tracers (e.g. $^{2}H_{H2O}$, $^{18}O_{H2O}$, Cl, ^{37}Cl, Br, He, Ar) in the pore-water of argillaceous formations have been investigated in profiles across several formations (FEPs 17 and 24; e.g. Couche silteuse at Marcoule/Gard, Callovo-Oxfordian at Bure, Toarcian-Domerian at Tournemire, Opalinus Clay at Mont Terri and at Benken). In many cases, curved distributions were observed and interpreted as diffusion profiles (FEP 8). Provided the initial and boundary conditions for the diffusion process can be constrained on the basis of independent information, modelling of such profiles potentially leads to the following conclusions:

- Assessment of the relative importance of diffusion and advection as transport processes. A maximum advective flux can be derived, beyond which the shape of the modelled tracer profiles would no longer fit the observed distributions. Typically, such advective fluxes are very small.
- Assessment of tracer-specific diffusion coefficients, referring to the spatial scale of the formation. These coefficients can be compared to those measured in the laboratory on small samples. Agreement among the two approaches would support the use of laboratory-measured diffusion properties of tracers not measured in the field for formation-wide calculations. That is, such agreement would support upscaling of laboratory results.

To date, different models and parameter sets were used at different sites, and a co-ordinated effort integrating information would improve the confidence in such models. The main issues could include:

- As in the case of hydraulic overpressures discussed above, the same model should be able to explain the existence of bell-shaped profiles for some tracers and the absence of such profiles for other tracers at a given site.
- Application of the same model to different sites should lead to consistent results (even though different parameter sets, e.g. diffusion coefficients and initial and boundary conditions may be needed). Again, the models should explain both the presence of curved diffusion profiles at one site and profiles without a spatial variation of tracer concentration (or isotopic ratio) at another site.
- There should be consistency in diffusion properties from site to site, taking into account differences in site characteristics such as pore-fluid salinity, formation mineralogy, porosity, compaction, etc.

A co-ordinated study aimed at the interpretation of tracer profiles would require comparable databases at all sites. Some data may be missing at present and should be acquired in a first step (e.g. complete tracer profiles, characterisation of initial and boundary conditions, laboratory-derived diffusion coefficients).

7.3 Geochemical stability

While many argillaceous formations have demonstrably very low hydraulic conductivities, which result in very small advective fluxes, diffusive fluxes may be more substantial over relatively short geological time scales. As an example, Cl contents of pore-waters in argillaceous units of the Benken borehole (Opalinus Clay and underlying Liassic) can be shown to have decreased by a factor of *ca.* 3 within 1-2 Ma close to the contact with the underlying aquifer. Exchange processes between pore-waters in argillaceous formations and embedding aquifers are relevant topics both for the future evolution of hydrochemistry (FEP 52) and the understanding of present-day pore-water compositions (FEP 17). Modelling of such exchange processes could contribute to our current understanding of controls of pore-water chemistry, buffering capacity (FEPs 17, 27) and thus the geochemical stability of the host formations.

Pore-waters in argillaceous rocks are typically in chemical equilibrium with the minerals present in the formation. The geochemical stability of the formation and its pore-water can be altered by changes in such boundary conditions as pressure, temperature and the pore-water chemistry of adjacent formations. Changes in boundary conditions may result from regional tectonic or erosional changes or other processes such as salt-water intrusion in near-coastal sites. These will be reflected by changes in the pore-water chemistry (and possibly the mineralogical properties) of a formation. The rates of change of these conditions for a site can often be evaluated from the geologic history of the region and (or) from modelling profiles of chemical tracers, as described above. The immediate past rate of change in formation chemistry may be applicable to the immediate future as well and so be useful in developing a base-case scenario for site evolution for PA.

An added contribution to the geochemical stability of argillaceous rocks is that they are chemically rock-dominated. That is, the majority of the chemical species dissolved in pore-water are buffered by minerals. The combination of fine grain size and extended pore-water residence times typical of argillaceous rocks assures that changes to pore-water chemistry that might be brought about by repository construction or operation will be strongly buffered by rock-water reactions. For example, this aspect of the Opalinus Clay at Mont Terri is described in FEP 27 with particular relevance to its redox buffer capacity.

7.4 Understanding diffusion

Diffusion is an important transport process in all types of argillaceous rocks and must be included in any PA involving such materials. In unfractured systems, diffusion is likely to be the dominant transport mechanism. In rocks where advective flow and transport may occur in fractures, diffusion from fracture to matrix fluid is an important retardation mechanism.

There is substantial evidence that Fick's laws of diffusion also apply to argillaceous systems, and so in most PAs, these laws are used to describe diffusion of solutes. The empirical description of diffusion by means of Fick's laws is currently considered to be state-of-the-art and sufficient for PA purposes.

Efforts are being made to develop mechanistic explanations for differences between predictions made using classical diffusion theory and observations of transport in materials with charged surfaces, large specific surface areas and very small pores. Many of these approaches are not sufficiently advanced and robust to be used in PAs. The following model approaches can be envisaged to quantify the total diffusive flux:

(a) A partitioned porosity approach in which it is assumed that electrostatic forces limit the movement of ions within the "ion-accessible" part of the total porosity. This approach invokes a diffusion-accessible porosity for each ion, depending on valence and hydrated ion size. Measurement of effective diffusivity is made using non-sorbing tracers, and the diffusive flux of sorbing tracers is calculated using distribution coefficients from batch sorption tests or from expert elicitation. This route has been contested by Oscarson (1994). The difficulty lies in determining the relevance of parameters measured in batch sorption tests to retardation measured in laboratory or field diffusion tests.

(b) Complex calculations of ion transport in the electrolyte between narrowly-spaced charged mineral surfaces, using an analytical model based on double-layer theory, or by using Monte Carlo simulation (and assumed pair-potentials). These are process models that are not suitable for use in PA.

(c) A parallel pathway approach in which a simple subdivision of the medium is proposed. This approach is pursued in Finnish studies to describe transport in compacted bentonite (e.g. Lehikoinen 1999). It postulates a subdivision into surface pathways and pore channels with an arbitrary boundary between the near-surface region, where “surface diffusion” is postulated, and the pores. In reality the activation energy for diffusion probably varies with distance from surface, approaching the activation energy for bulk liquid viscosity at some distance. In the Finnish approach, the postulated numerical relationships assume that the cross-sectional area for surface diffusion is the same as the cross-sectional area of the mineral solids. The surface diffusion coefficient is therefore a phenomenological constant with no fundamental significance.

(d) The average flux approach, based on direct laboratory measurements (diffusion tests) which incorporate sorption. This is the simplest and most useful approach to PA, but it is very demanding in terms of experimental effort. Even for moderately sorbing solutes, this approach leads to difficulties in the interpretation of the experimental results because only small diffusion depths are possible within laboratory time scales. On the other hand, there is no need to worry about surface diffusion, since all possible mechanisms are incorporated in the measurements.

(e) For formations with suitable physical properties (e.g. high enough hydraulic conductivities and sufficient plasticity), diffusion coefficients and diffusion porosities can be found from a series of laboratory pulse injection experiments (Put, 1985, Put *et al.*, 1991, Aertsens e*t al*, 2003).

(f) The electromigration approach uses an electrical field to force ions to move towards the electrode of opposite charge. From these experiments the apparent diffusion coefficient is obtained. Compared to the classical methods (through diffusion, percolation), this method decreases spectacularly the experimental time which is especially interesting for the study of strongly sorbed species (Maes *et al*., 1998, 1999, 2001, 2002). Because transport phenomena other than just diffusion (such as electro osmosis) may also act in such experiments, it may be necessary to "validate" the technique with the results of classical diffusion experiments with samples of the same type of rock.

Approaches to constrain diffusion properties based on the measurement of electrical conductivity were also developed (e.g., Conca & Wright, 1990, 1991, Conca *et al.*, 1993). Such approaches were mostly used for unsaturated rocks, and no experience is available for saturated argillaceous rocks.

A recent report by Bradbury & Baeyens (2002) shows good agreement between the diffusivities obtained from diffusion tests (approach d) and diffusivities derived from distribution coefficients measured in batch sorption tests (approach a) for Cs(I), Ni(II), Sm(III), Am(III), Zr(IV) and Np(V). It was important in this comparison to properly adapt the distribution coefficients to the relevant pore-water composition. This report does not entirely solve the problems of compatibility between approaches (a) and (d) because it reports that for other elements less favourable agreement was observed. FEPs 8 through 11, the A1.2 (Diffusion) and A2.1 (Retardation mechanism) series, address parameters and processes that should be considered when evaluating various approaches to establishing parameters used to calculate diffusive fluxes for PA.

7.5 Understanding sorption

Sorption in the broad sense refers to the partitioning of a substance between solid phase(s) and solution. Due to sorption, the transport rate of the bulk substance is retarded relative to the rate of movement of the solution. There is a large amount of empirical evidence that sorption on mineral surfaces occurs, among others on clay minerals. Sorption is commonly included in PA using the distribution coefficient (K_d) parameter. K_d values vary by substance, substrate and solution properties. They can be derived from laboratory measurements using material from the formation of interest, or individual minerals typical of those in the host rock. Alternatively, they can be calculated from D_e and D_a values of the formation (FEP 8). For simple systems, approaches exist or are being developed to model sorption based on mechanistic principles, although this is not (yet) feasible for more complex systems.

To extend laboratory data and justify their application in differing PA environments, Altmann & Bruno (2001) describe a process-based interpretation of sorption, the Thermodynamic Sorption Model (TSM). This model treats sorption in terms of two component processes: ion exchange (FEP 20) and surface complexation (FEP 21). An important purpose of such a process-based interpretation is to build confidence in the use of simplified, empirical parameters, such as K_d values to describe sorption processes.

Because of its high clay-mineral content, the number of ion exchange sites in a typical argillaceous rock far exceeds the number of surface complexation sites, although the latter tend to bond more strongly to solutes of interest in PA than do the former. Ion exchange reactions are well understood and characterised insofar as they influence the major ion chemistry of pore-waters. Mechanistic modelling of reactions controlling the sorption of trace elements, whether treated formally as ion exchange or surface complexation reactions, works sufficiently well for pure substances such as metal oxides and hydroxides or clay minerals in simple solutions. The application of mechanistic models to complex systems, however is, still a difficult task.

Davis *et al.* (1998) examine two techniques for applying the surface complexation model to predict K_d values for natural systems with mineralogy and water chemistry of normal field complexity:

- In the first, termed Component Additivity (CA), the densities of sites corresponding to a number of specific sorbents are determined. The stability constants and reactions associated with each specific sorbent are known from laboratory studies and the overall sorption is predicted as the sum of the sorption corresponding to each site.
- The second technique is called the Generalised Composite (GC) method. Here, laboratory sorption measurements on the bulk host rock are made by using artificial pore-waters with compositions spanning those expected in the environment to be modelled. These results are simulated using the simplest surface complexation model that provides an acceptable fit to the laboratory data. Because the experimental data bracket the environmental conditions, the simulation will be applicable to the field problem.

Davis *et al.* (1998) compare the two methods for a system in which sorption occurs on mineral oxide and hydroxide coatings. The site densities of these coatings could not be characterised precisely enough for the CA method to yield results comparable to those of the GC method.

On the other hand, Bradbury & Baeyens (1997, 2003) employ a method analogous to the CA method using a series of conversion factors to generate K_d values for the Palfris Formation and for Opalinus Clay from the properties of its components. Their results are in generally good agreement with results of the GC method, presumably because the sorption capacity of the formation is due principally to ion exchange and surface sites of illite and mixed-layer smectite-illite, the quantities of which can be determined with acceptable precision.

The ongoing NEA Sorption Project aims at maintaining consistency among different national programmes and to co-ordinate various modelling approaches. The objective of Phase II of this project is to demonstrate the applicability of different thermodynamic modelling approaches to support the selection of sorption parameters for PA. First results of this work are documented in Payne *et al.* (2003) and Davis *et al.* (2003).

The difficulties associated with the upscaling of laboratory data are recognised and are being addressed by field studies in underground research laboratories, by studies of trace element transport from conventional waste disposal sites, such as that of Davis *et al.* (1998), and in laboratory and theoretical studies in support of many national nuclear waste programmes to improve mechanistic understanding.

7.6 Time evolution and geometry of the EDZ, self-sealing

In geotechnical and mining engineering, the evolution and geometry of the “Plastic Zone” as part of an EDZ is a key issue in the design of tunnels and other underground openings. Many theories have been developed, but the availability of appropriate data is still a major issue. In-depth information from various underground research laboratories constitutes a very valuable set of much needed new *in situ* data. Moreover, purpose-designed innovative tools were developed which enable an accurate delineation of the geometry, extent and evolution of the plastic zone. An example is the Interval Velocity Measuring Method in boreholes developed by Alheid and co-workers, which was employed e.g. in Tournemire and Mont Terri (Schuster *et al*., 1999). The investigations carried out in the New Gallery of the underground research laboratory at Mont Terri revealed the extent and degree of fracturing of the EDZ and the changes with time in a detail which, in the opinion of the Expert Group, is without precedent in underground construction.

The evolution of the EDZ after repository closure is affected by a number of processes, such as resaturation, pressure build-up, swelling and disintegration/homogenisation on a nanometric scale. These processes contribute to self-sealing, i.e. the reduction of hydraulic conductivity of fractures with time. Self-sealing is of key importance to PA and is often cited as an important factor favouring the choice of argillaceous formations as host rocks for deep disposal. Self-sealing directly addresses the functionality of the argillaceous host rocks as a migration barrier. When the self-sealing process proceeds in reasonable time, fractures created by the construction of the repository will not persist as preferential pathways for radionuclide migration, and thus the system becomes diffusion-dominated.

Self-sealing also occurs in natural fractures and faults penetrating argillaceous rocks. Substantial evidence exists that natural fractures are not hydraulically active and have not been active over geological periods of time. In Swiss railway tunnels (>100 years old) in the Jura Mountains, no water inflows were observed at an overburden >200 m, in spite of the presence of major faults. Evidence from other sites is consistent with this observation. This set of observations constitutes a strong geological argument for the self-sealing capabilities of argillaceous formations, addressing both sealing of natural fractures as well as the EDZ around underground openings.

Self-sealing mechanisms have been widely observed in a variety of argillaceous rocks, and the basic physico-chemical and hydro-mechanical processes leading to self-sealing are well understood. In plastic clays, self-sealing is expected to be a rather quick process. In more indurated argillaceous rocks, self-sealing is expected to be slower. However, the currently available knowledge is not yet sufficient to permit detailed predictions concerning the kinetics of the self-sealing process in various types of argillaceous media.

In spite of the existing data and observations, understanding still needs to be improved. One question is whether the observed self-sealing of natural fractures can be extrapolated to the sometimes geometrically different fracture arrays in an EDZ. Wedge-shaped and composite fracture planes, for instance, may develop in the roof of tunnels excavated in horizontally bedded argillaceous rocks. For this case geological analogues may be of limited value, as natural and EDZ fracture planes may be different in shape. The resistance to closure of composite and wedge-shaped fracture planes, particularly in response to swelling pressures originating in the formation and/or in the backfill, should be carefully investigated. Such questions can be addressed by experiments in underground research laboratories, such as the EC SELFRAC project. In this project, *in situ* experiments studying the kinetics of the self-sealing process have only recently been conducted at Mol and at Mont Terri. It would also be interesting to study self-sealing in more strongly indurated formations, such as in the Toarcian-Domerian at Tournemire.

Besides the hydro-mechanical evolution of the EDZ, chemical reactions may occur in the EDZ during the operational phase of the repository. For example, EDZ fractures create pathways for oxygen. The most relevant chemical effect is the oxidation of pyrite, which occurs as an accessory phase in all formations considered (except for the Boda Clay Formation). There is substantial evidence that pyrite oxidation will not have detrimental effects on the geochemical and geomechanical properties of the EDZ. Evidence from laboratory experiments and from natural analogues (such as tunnels penetrating argillaceous formations or surface-near decompaction fractures) indicates that oxidation penetrates only a few cm into the rock matrix even if exposure to air occurs over decades. The acid produced due to pyrite oxidation will be consumed by a small degree of calcite dissolution, thus pH will be buffered by the carbonate system and will not drop substantially (all formations considered contain calcite). As the EDZ self-seals, the access of oxygen to the rock gets blocked. Thus the kinetics of the self-sealing process will influence the magnitude of oxidation and, by consequence, the geochemistry in the affected field of the repository.

7.7 Present-day stress regime

In most answers to the questionnaires, the present-day (geologic) stress regime is generally acknowledged to be a relevant FEP (see Section II, Chapter 55). On the other hand, the questionnaires also show that problems commonly exist in the experimental determination of the site-specific *in situ* stress state in argillaceous rocks, and meaningful conclusions need to be based on a variety of individual measurements and observations. At Mont Terri, for instance, even a combined application of various standard stress-measuring techniques (overcoring; undercoring; borehole slotting; hydraulic fracturing) did not reveal a reasonably coherent picture of the local geologic stress regime. It was only after the back-analysis of the deformational behaviour of the excavations of the underground rock laboratory that a consistent picture emerged. Similarly, at other sites, additional evidence had to be considered to interpret *in situ* stress measurements with confidence. Such evidence may consist of either geologic stress indicators (e.g. stylolites; orientation of volcanic dykes, faults or joints) or technical stress indicators (e.g. borehole breakouts; spalling of tunnel walls; orientation of blast hole fractures).

Obviously, argillaceous rocks constitute an “intermediate” material in which neither the standard stress measuring techniques originally developed for hard rocks (e.g. the above-mentioned methods) nor those developed for soft soils (e.g. total pressure cell inclusions) are easily applicable. In argillaceous materials it is often difficult to provide well-shaped cylindrical boreholes (which are required e.g. in hydro-fracturing and overcoring). The borehole wall itself is commonly disturbed and fractured. The rock close to the borehole wall thus does not necessarily behave in a linear-elastic way, which is one of the pre-requisites for under- and overcoring as well as for borehole slotting stress measuring tests. Against the background of these conceptual and technical difficulties, it appears meaningful to review the usefulness of the various *in situ* stress measuring methods in argillaceous materials in a more systematic manner and to pursue a special programme for the adjustment and/or the development of *in situ* stress measuring techniques, if required.

7.8 Conceptual micro-mechanical models

The number and application fields of conceptual micro-mechanical models as specified in the answers to the questionnaires are quite remarkable, if not surprising. Examples of micro-mechanical modelling were mentioned in connection with FEPs 37 (Geomechanical rock properties) and 47 (Gas migration through stress-induced porosity). Other applications include the modelling of compaction (FEP 50) and self-sealing (FEP 42) processes.

Since the formulation of the “effective stress principle” (Terzaghi, 1925), it is generally acknowledged that micro-mechanical models are keys for an in-depth mechanical understanding of soils and rocks and for the prediction of their thermo-hydro-mechanical response to forces in space and time. Comprehensive formulations of material behaviours by means of micro-mechanical models require the determination of a vast number of parameters as well as the consideration of numerous interaction processes. In most standard applications, micro-mechanical modelling was and still is considered to be impractical. However, with the advent of powerful micro-mechanical numerical modelling codes (e.g. PFC – Particle Flow Code of the Distinct Element Method) and driven by the steadily increased computing power, the situation is rapidly changing. This, for instance, is documented in Konietzky (2003), where ample evidence is provided that, beyond geomechanics, micro-mechanical modelling is successfully carried out in scientific fields and applications as diverse as process engineering, chemical industry, material science, agriculture and mechanical engineering.

The FEPs compilation indicates that micro-mechanical modelling became a realistic perspective for argillaceous rocks. Such modelling has the potential to adequately describe and predict geomechanical phenomena which are often intractable in conventional generic-type mechanical models. Examples of such phenomena are time-dependent deformation (“creep”), the development of shear bands and the clustering of particles. Particularly with regard to the mechanisms which may lead to “secondary creep” in argillaceous rocks, it is, in the opinion of the Expert Group, desirable to carry out further systematic micro-mechanical modelling studies to enhance understanding of the relevant processes. When addressing PA-relevant time scales, upscaling in space and time (as discussed in Section I, Chapter 7.1) is needed for experiments carried out in laboratories or underground research laboratories. For example, the upscaling of creep requires some understanding of the underlying physico-chemical mechanisms and processes on a microscopic scale.

8. CLASSIFICATION OF FEPS ACCORDING TO STATE OF KNOWLEDGE AND POTENTIAL RELEVANCE FOR PERFORMANCE ASSESSMENT

The full FEPs compilation (Section II of this report) addresses, among other issues:

- the scientific and PA-related state of knowledge on each FEP; and
- the relevance of each FEP for PA (or, more broadly, for a safety case).

In Table 7, this information has been summarised and classified in a small number of categories. Even though this is a simplification of a highly complex situation, it may be used by each national organisation as a potential checklist to qualify its own progress in a disposal project. However, the table must not be mistaken as a universal rating for the following reasons:

- The relevance of a FEP for a disposal project depends on system-specific requirements and boundary conditions (e.g. type of waste, disposal concept, type of engineered barriers). Some FEPs might be of importance in one concept but not an issue in another.
- Some FEPs that could be relevant for radionuclide transport can be neglected if it can be shown that disregarding them leads to an overestimation of calculated doses. For example, the low-permeability formations embedding the Opalinus Clay in the Zürcher Weinland were characterised to a less detailed degree than the host formation itself. In the radionuclide transport calculations, retention in these units was not considered in the base case, which is a simplification leading to higher calculated doses.
- The degree of knowledge on a FEP varies among disposal projects at different stages of maturity (regional or generic feasibility study, site-specific work from the surface, site-specific underground research laboratory, etc.).

Each FEP was classified according to the following simple scheme:

Classification	Meaning	Consequences from a PA perspective
1	FEP is potentially PA-relevant. There is a general consensus that it can be adequately characterised in terms of processes and parameters.	Methods and tools are available for a sufficient quantitative understanding.
2	PA relevance and/or the degree of knowledge are heterogeneous for different programmes and disposal concepts.	PA relevance to be established, adequate characterisation needed at least in some programmes and repository concepts.
3	There is no general consensus on the potential relevance of the FEP for PA and/or the adequacy of its characterisation in specific programmes and repository concepts.	
4	FEP is of low PA relevance, even though it is well characterised.	No urgent actions needed.
5	FEP is of low PA relevance. The degree to which is characterised is variable at different disposal sites. At least in some cases, knowledge is quite limited.	

Classifications 1, 4 and 5 mean that data and understanding are either available or not necessary from a PA perspective. Classifications 2 and 3 mean that knowledge may be limited at least for some programmes and disposal concepts, in spite of a potential PA relevance. For some of these FEPs, there is a potential for future actions on a national or international level. However, it must be stressed that even FEPs classified as 2 or 3 may be non-issues for some programmes and disposal concepts, and the fact that they have been assigned these codes must not be mistaken as general prompts for new actions.

The following specific points can be made:

- The degree to which a FEP has been characterised at different sites is highly variable. In many cases, methods and tools leading to good knowledge for a FEP are available but were not applied at all sites. In such cases, knowledge was rated as being good in Table 7. Each participating organisation can judge its own level by consulting the compilation in Section II.
- In Table 7, different classifications are listed for advection-dominated and diffusion-dominated systems. A number of FEPs that are important in advection-dominated systems are not relevant for diffusion-dominated systems. Thus a larger number of FEPs needs to be considered for advection-dominated systems. In principle, all sites except the Palfris Formation at Wellenberg (Switzerland) and the Boda Clay Formation (Hungary) can be considered to be diffusion-dominated. However, the irrelevance of continuous or

episodic fracture flow cannot be proven in some cases, and so fracture flow is assumed at least in alternative scenarios of PA.

- Upscaling in space and time is an issue for a number of FEPs and a source of uncertainty (see Section I, Chapter 7.1).
- The number of completed questionnaire answers received for a FEP is also listed in Table 7. While it clearly is not an absolute measure of the state of knowledge, it may provide some indications.

Table 7. **Classification of FEPs according to state of knowledge and PA relevance**

FEP no		Number of quest. answers	FEP name	Availability of PA-relevant knowledge on FEP	Relevance of FEP for PA (or, more generally, a safety case)	Classification for diffusion-dominated systems	Classification for advection-dominated systems
1	A1.1	7	Advection/dispersion	Good for matrix flow, more limited for fracture flow	Important transport process with limited consequences in diffusion-dominated systems (applies to most sites investigated), highly relevant in advection-dominated systems with fracture flow	**1**	**2**
2	A1.1.1	8	Size and geometry of the host rock and of surrounding units, migration path length	Good	High	**1**	**1**
3	A1.1.2	6	Migration pathways, including heterogeneity and anatomy	Sedimentary structures well known; database for tectonic structures and their hydraulic significance is limited, and upscaling in space and time may be problematic mainly in highly indurated formations where fracture flow could be important. However, they can often be avoided by design.	High	**1**	**2**

FEP no		Number of quest. answers	FEP name	Availability of PA-relevant knowledge on FEP	Relevance of FEP for PA (or, more generally, a safety case)	Classification for diffusion-dominated systems	Classification for advection-dominated systems
4	A1.1.3	5	Undetected geological features	Currently variable, but can be much improved by applying available techniques (e.g. 3-D seismics).	Limited in diffusion-dominated systems (due to the expected hydraulic irrelevance of undetected features), more relevant in highly indurated, advection-dominated systems with fracture flow (higher degree of heterogeneity).	**1**	**2**
5	A1.1.4	10	Hydraulic potentials and gradients in the host rock, including boundary conditions	Generally good (except for the understanding of abnormal pressures)	Necessary input for quantifying advection, which is an important transport process. Its consequences are limited in diffusion-dominated systems (applies to most sites investigated), but it is relevant in advection-dominated systems with fracture flow.	**1**	**1**
6	A1.1.5	10	Hydraulic properties of the host rock	Good, except for spatial upscaling (namely in systems where fracture flow dominates)	High	**1**	**2**
7	A1.1.6	5	Units over- and underlying the host formation: local and regional hydrogeologic framework	Good	High	**1**	**1**
8	A1.2.1 A2.1.1	11	Diffusivity	In general good, more limited for retarded species	High	**1**	**1**
9	A1.2.2 A2.1.2	8	Connected matrix porosity	Good	High	**1**	**1**
10	A1.2.3 A2.1.4	4	Ion exclusion	Good	High	**1**	**1**
11	A1.2.4 A2.1.5	3	Surface diffusion	Limited	Limited, if any at all	**5**	**5**
12	A1.3	3	Colloid formation, transport and filtration	Limited, but the functionality of the matrix of argillaceous rocks as a colloid filter is established.	Limited in diffusion-dominated systems, relevant in advection-dominated systems with fracture flow	**4**	**3**

FEP no		Number of quest. answers	FEP name	Availability of PA-relevant knowledge on FEP	Relevance of FEP for PA (or, more generally, a safety case)	Classification for diffusion-dominated systems	Classification for advection-dominated systems
13	A2.1.3	2	Flow-wetted surface and accessibility of matrix	Fair	Irrelevant in diffusion-dominated systems, more relevant in advection-dominated systems with fracture flow	**4**	**2**
14	A2.2.1	7	Lithology, mineralogy of rocks and fracture infills	Good	High	**1**	**1**
15	A2.2.2	6	Natural organics, complexation	Fair	Variable (depending on the nature of the organic matter involved and the nuclide inventory); complexation: high	**2**	**2**
16	A2.2.3	2	Mineral-surface area	Good	High	**1**	**1**
17	A2.2.4	6	Pore- and fracture water composition	Good except for 1) modelling uncertainty and 2) distinction between fracture and matrix water.	High	**1**	**2**
18	A2.2.5	3	Dissolution/precipitation of solid phases	Major phases: good; phases limiting solubilities of radionuclides: limited.	High (solubility limits of radionuclides)	**2**	**2**
19	A2.2.6	1	Solid solutions/co-precipitation	Moderate; can be modelled in principle.	Potentially high, often (conservatively) neglected	**2**	**2**
20	A2.2.7	4	Ion exchange	Good; can me modelled in principle but data are limited.	High	**1**	**1**
21	A2.2.8	5	Surface complexation	Fair (empiric data sufficient, mechanistic understanding limited)	High	**2**	**2**
22	A2.2.9	5	Thermodynamic and kinetic modelling data	Variable (depending on element)	High	**2**	**2**
23	A3.1 C1.1.1	4	Palaeo-hydrogeology of the host formation and of embedding units	Good in principle even though not available in full at all sites	High	**1**	**1**
24	A3.2 C1.1.2	5	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units	Good in principle even though not available in full at all sites	High	**1**	**1**
25	A3.3	5	Water residence times in the host formation	Good in principle even though not available in full at all sites	High	**1**	**1**

FEP no		Number of quest. answers	FEP name	Availability of PA-relevant knowledge on FEP	Relevance of FEP for PA (or, more generally, a safety case)	Classification for diffusion-dominated systems	Classification for advection-dominated systems
26	B1.1	4	Oxidation of the host rock	Good	Variable; depends on formation, repository design and operation	**1**	**1**
27	B1.1.1	1	Redox buffering capacity of the host rock	Good, but reaction rates are difficult to measure	Variable (system dependent)	**2**	**2**
28	B1.2	0	Effects of repository components on pore-water chemistry in the host rock	Limited (no questionnaire answers received)	Effects are expected to be spatially limited in diffusion-dominated systems; otherwise not well established.	**2**	**3**
29	B1.2.1	4	Interactions of hyperalkaline fluids and host rock	Fair (but the issue is complex)	Effects are spatially limited at least in diffusion-dominated systems; potentially relevant in advection-dominated systems.	**1**	**2**
30	B1.2.2	4	Organics from waste and their effect on transport properties of the host rock	Limited	Effects are spatially limited at least in diffusion-dominated systems; otherwise not well known due to the scarcity of information.	**2**	**3**
31	B2.1	3	Thermal effects on mineral stability and pore-water composition	Fair	Limited	**4**	**4**
32	B2.2	7	Thermal rock properties	Good	High	**1**	**1**
33	B2.3	3	Thermally induced consolidation of the host rock	Limited	Limited	**5**	**5**
34	B3.1	6	Geomechanical stability	Good	Limited for PA but important for the safety concept	**1**	**1**
35	B3.2	6	Size and structure of the EDZ	Fair	High	**2**	**2**
36	B3.3	2	Effects of bentonite swelling on the host rock	Good, except for scarcity of experimental data and understanding of closure mechanisms of fractures, mainly in systems with fracture flow	High	**1**	**1**
37	B3.4	6	Geomechanical rock properties	Variable (depending on site/programme)	High (repository concept and PA)	**2**	**2**

FEP no		Number of quest. answers	FEP name	Availability of PA-relevant knowledge on FEP	Relevance of FEP for PA (or, more generally, a safety case)	Classification for diffusion-dominated systems	Classification for advection-dominated systems
38	B4.1	5	Hydraulic properties of the EDZ	Fair (upscaling of measurements in space and time is difficult)	High	**2**	**2**
39	B4.2	4	State of saturation of the EDZ and desiccation cracking	Fair	Limited	**4**	**4**
40	B5.1	5	Coupled thermo-hydro-mechanic processes	Generally good (but the issue is complex due to the large number of possible couplings and due to limitations in the site-specific parameter sets)	Probably limited, but currently difficult to judge	**2**	**2**
41	B5.2 C2.3	3	Swelling	Fair (good generic understanding, limitations in site-specific data sets)	High	**2**	**2**
42	B5.3 C2.4	3	Self-sealing	Fair (good generic understanding, limited site-specific quantitative information)	High	**2**	**2**
43	B5.4	3	Off-diagonal Onsager processes except chemical osmosis	Limited	Limited	**5**	**5**
44	B5.5	3	Chemical osmosis	Fair	Limited for PA; potentially high for system understanding in some cases	**2**	**2**
45	B6.1	2	Gas dissolution and chemical interactions between gas and pore-water	Good	High	**1**	**1**
46	B6.2	5	Gas migration through the primary porosity (matrix, natural fractures)	Fair (upscaling difficult)	Limited to high (system-dependent)	**2**	**2**
47	B6.3	5	Gas migration through stress-induced porosity (gas fracs, pathway dilation)	Fair (good qualitative understanding, quantification and uscaling difficult)	Limited to high (system-dependent)	**2**	**2**
48	B6.4	2	Gas-induced transport in water	Limited to fair (upscaling and parametrisation are difficult)	Probably limited, even though no detailed models are available	**2**	**2**
49	B7	2	Microbiological perturbations	Limited	Unclear; limited in the unfractured matrix due to space constraints	**3**	**3**

FEP no		Number of quest. answers	FEP name	Availability of PA-relevant knowledge on FEP	Relevance of FEP for PA (or, more generally, a safety case)	Classification for diffusion-dominated systems	Classification for advection-dominated systems
50	C1.1.3	6	Past burial history	Good (not at all sites)	High	**1**	**1**
51	C1.2.1	4	Present and future geothermal regime and related processes	Fair to good	Limited for systems and time scales considered in FEPCAT	**4**	**4**
52	C1.2.2	3	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)	Limited to good (depends on site)	Limited for diffusion-dominated systems, more important for advection-dominated systems with fracture flow	**5**	**2**
53	C2.1	2	Past deformation events	Fair (not available in full at all sites; dating of deformation events is difficult)	High (important for understanding geometries and future scenarios)	**2**	**2**
54	C2.2	3	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events	Limited to fair	Limited for diffusion-dominated systems, more important for advection-dominated systems with fracture flow	**5**	**2**
55	C2.5	5	Present-day stress regime	Good (even though not for all sites)	Important for repository design and safety concept	**1**	**1**
56	C2.6	0	Future stress regime	Good over the time scales considered in FEPCAT	Potentially high if overburden thickness changes substantially	**1**	**1**
57	C3.1	4	Geomechanical effects of erosion / unloading	Fair (good conceptual basis)	Potentially high if overburden thickness is reduced substantially	**1**	**1**
58	C3.2	2	Consolidation due to burial	Fair	Limited over the time scales considered in FEPCAT	**4**	**4**
59	C3.3	7	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)	Fair (good conceptual basis)	Limited to high, site-specific. Possibly relevant in advection-dominated systems.	**4**	**2**

9. CONCLUSIONS

9.1 Project management

Due to its very wide technical scope (geology, geochemistry, hydrogeology, rock mechanics) and aspects covered (from *in situ* and laboratory-based data acquisition to interpretation and application in PA), the FEPCAT project was very demanding for both the Expert Group and the participating national organisations. The initial planning was very ambitious, and the necessary efforts were underestimated. The initial objectives of the project could only be fulfilled by investing more resources and time than originally foreseen.

The total number of answers to the questionnaires was limited. Out of *ca.* 600 possible answers, 224 were obtained from the participating organisations. While some FEPs are well documented, only very limited information was provided for many others. One reason (out of several) for this limitation is the ambitious structure and number of questions asked in each questionnaire form. In retrospect, a less demanding questionnaire structure might have generated a more substantial feedback.

It is recognised that work for the FEPCAT project, both within the participating organisations and within the Expert Group, stimulated communication between representatives of different scientific disciplines, and between field researchers and engineers dealing with PA aspects.

9.2 Technical insights

9.2.1 General

Out of the participating organisations, only a minority have a safety case in argillaceous rocks. On the one hand, this fact illustrates the necessity and usefulness of FEPCAT-type initiatives. On the other hand, this limits those aspects of the answers to the questionnaire that address the linkage of site characterisation and performance assessment. Gaps in addressing these aspects were reduced by knowledge available within the Expert Group, by personal interviews and by consulting background literature.

In a number of fields, NEA publications were the most useful literature references (e.g. EDZ, link hydrochemistry/hydrogeology). The more focussed the theme of NEA publications, the more useful they were for FEPCAT.

9.2.2 The FEPs list

The FEPs list was derived by combining two approaches, namely the collection of FEPs available in the literature (BOGSAT approach) followed by a process-oriented structuring (top-down approach). A variety of screening criteria were applied to derive the final FEPs list with 59 entries out of an original list with more than 500 FEPs. There is a general agreement that the proposed FEPs list is appropriate, i.e. it is complete (vis-à-vis the scope of the project) and still short enough.

9.2.3 State of knowledge and relevance of all FEPs in the FEPs list

On the basis of the FEPs compilation, FEPs were judged according to the degree to which they are understood in qualitative and quantitative terms, and according to their relevance in PA. Even though such judgements include some degree of subjectivity and also may vary between host rocks and repository designs, they are regarded as useful tools guiding future activities. Table 8 summarises those FEPs which are regarded relevant but not fully understood in diffusion-dominated argillaceous systems. For advection-dominated systems with fracture flow, understanding is required for a larger number of FEPs. Table 8 and Table 9 combined include all FEPs where more understanding is required when considering advection-dominated systems.

Table 8. **Classification of FEPs according to state of knowledge and PA relevance: Selection of those FEPs that are regarded as relevant but not sufficiently well understood in diffusion-dominated systems (codes 2 and 3). See above for explanation of classification codes.**

FEP no.	FEP name	Classification
15	Natural organics, complexation	2
18	Dissolution/precipitation of solid phases	2
19	Solid solutions/co-precipitation	2
21	Surface complexation	2
22	Thermodynamic and kinetic modelling data	2
27	Redox buffering capacity of the host rock	2
28	Effects of repository components on pore-water chemistry in the host rock	2
30	Organics from waste and their effect on transport properties of the host rock	2
35	Size and structure of the EDZ	2
37	Geomechanical rock properties	2
38	Hydraulic properties of the EDZ	2
40	Coupled thermo-hydro-mechanic processes	2
41	Swelling	2
42	Self-sealing	2
44	Chemical osmosis	2
46	Gas migration through the primary porosity (matrix, natural fractures)	2
47	Gas migration through stress-induced porosity (gas fracs, pathway dilation)	2
48	Gas-induced transport in water	2
49	Microbiological perturbations	3
53	Past deformation events	2

Table 9. **Classification of FEPs according to state of knowledge and PA relevance in advection-dominated systems. FEPs that are regarded as relevant but not sufficiently well understood (codes 2 and 3) correspond to the sum of Tables 8 and 9 (i.e. Table 9 only lists those FEPs that are classified differently for diffusion-dominated and advection-dominated systems). See above for explanation of classification codes.**

FEP no.	FEP name	Classification
1	Advection/dispersion	2
3	Migration pathways, including heterogeneity and anatomy	2
4	Undetected geological features	2
6	Hydraulic properties of the host rock	2
12	Colloid formation, transport and filtration	3
13	Flow-wetted surface and accessibility of matrix	2
17	Pore- and fracture water composition	2
28	Effects of repository components on pore-water chemistry in the host rock	3
29	Interactions of hyperalkaline fluids and host rock	2
30	Organics from waste and their effect on transport properties of the host rock	3
52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)	2
54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events	2
59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)	2

9.2.4 Advection-dominated vs. diffusion-dominated argillaceous systems

The majority of all sites in argillaceous rocks under investigation for waste disposal purposes are considered diffusion-dominated with fracture flow most likely irrelevant. Major efforts were and are being made to clearly demonstrate the hydraulic insignificance of fractures and the efficiency of self-sealing processes. As shown in Table 8 and Table 9, the number of FEPs that need to be considered (i.e. codes 2 and 3) for diffusion-dominated systems is smaller than for advection-dominated systems.

However, even in formations that are interpreted to be diffusion-dominated, fracture flow, whether continuous or episodic, may be considered in PA, mostly in the framework of “what if” calculations or alternative scenarios. The motivation for such PA calculations is to quantify the impact of fracture flow as a very conservative model assumption and/or to account for the uncertainty in the long-term evolution (e.g. possibility of transient flow events).

9.2.5 Constraining repository-derived perturbations

Apart from scaling issues, there are other, currently underused ways of applying the host formations as their own analogues. In some cases, FEPs relating to the far field can be used to constrain processes expected to occur in the host rock affected by the presence of the repository. Examples of such situations include:

- FEP 50 (Past burial history) can be used to put thermal perturbations derived from the repository into perspective. Specifically, FEPs 31 (Thermal effects on mineral stability and pore-water composition) and 33 (Thermally induced consolidation of the host rock) can be dealt with by comparing the thermal impact (maximum temperature and/or time-temperature integral) from the repository with the one experienced by the formation during natural burial.
- FEP 42 (Self-sealing) relates to a process that occurs both in natural fractures and faults and in the EDZ. Observations of self-sealing in natural systems provide constraints on the functionality of this process in the EDZ.

9.2.6 Scaling issues

For a substantial number of FEPs, scaling issues turned out to be relevant. While laboratory-based knowledge is good for many of these FEPs, uncertainties were identified in upscaling the information in space and time to the scales appropriate for PA. Promising techniques for upscaling include:

- *In situ* experiments in underground research laboratories (scales intermediate between laboratory and PA)
- Use of the host formation and its past evolution as its own natural analogue. Specifically, some far-field FEPs can be used for upscaling other FEPs. A complete list is given in Table 6.
- Employment of micro-mechanical models for identification and better understanding of relevant mechanisms (see Section I, Chapter 7.8).

9.2.7 Demonstration of low permeability and limited relevance of advection

Among the most promising examples of using the host formation as its own natural analogue are profiles of chemical parameters and hydraulic states across the formation. Modelling such profiles provides constraints on the following features and processes:

- hydraulic conductivity and vertical advective flux across the formation;
- diffusion constants (relevant for the spatial scale of the formation and for very long time scales);
- long-term evolution of the hydraulic and geochemical regime.

The quantification of chemical and hydraulic profiles requires independent information on initial and boundary conditions, i.e. on the evolution of the aquifers above and below the host formation. At many sites, the degree to which these conditions can be constrained is sufficient to obtain meaningful results and conclusions. At present, chemical profiles provide more quantitative information than hydraulic profiles because the measurement of pore-water pressures in low-permeability systems is lengthy and may be associated with substantial uncertainty.

9.2.8 Geochemical stability

Geochemical stability is one of the more attractive features of argillaceous host rocks. This stability is particularly evident in diffusion-dominated systems and has two aspects:

- Because of the fine grain size and relatively long residence times of water in such formations, chemical reactions of importance to solute transport are generally at equilibrium. Because the chemistry of reactive solutes is generally rock dominated, the rock – pore-water system is a robust buffer against repository-induced chemical changes.
- As pointed out in the previous chapter, the rate of evolution of the geochemical properties of many potential argillaceous host rocks can be shown to be very slow by interpreting such characteristics as the Cl distribution in the pore-water itself. Such interpretations show that argillaceous formations are also well-buffered against external geochemical changes.

9.2.9 Diffusion

Diffusion is the dominant solute transport mechanism in many argillaceous rocks and, through the mechanism of matrix diffusion, can also have a significant retarding effect on the rate of advective transport in fractures. Mechanistic understanding of the diffusion of reactive solute ions in charged porous media like clay-rich rock is limited but is sufficient to extend empirical data to support diffusion modelling for PA.

9.2.10 Sorption

Sorption of radio-elements and other solute ions contributes positively to the favourable transport properties of argillaceous rocks. Mechanistic interpretations in terms of ion exchange and surface complexation processes are useful for interpreting laboratory studies and for geochemical modelling of their major-ion chemistry. Solute transport models used to support PA are usually based on the bulk sorption properties of the formation described using distribution coefficient (K_d) values.

A better mechanistic understanding of the processes of ion exchange and surface complexation, which together determine the sorption properties of a formation, would add confidence to the time and space extrapolations of empirical sorption parameters that underlie some of the present generation of PA models.

9.2.11 Time evolution and geometry of the EDZ, self-sealing

Substantial progress in the structural and hydrogeological characterisation of the EDZ was achieved in recent years, namely due to *in situ* work in underground research laboratories and due to modelling efforts.

- The geotechnical feasibility of tunnelling in argillaceous rocks is undisputed. Detailed relationships between water content and geomechanical parameters have been elaborated.
- The geometry and evolution of the EDZ was recognised as a key issue for PA because it may directly affect the functionality of the repository system.
- Self-sealing is often cited as a primary factor favouring the choice of argillaceous formations as host rocks for deep disposal. Self-sealing mechanisms have been widely observed in a variety of argillaceous rocks, and the basic physico-chemical and hydro-mechanical processes leading to self-sealing are reasonably well understood. In plastic clays, self-sealing is expected to be a rather quick process compared to geological time scales. In more indurated argillaceous rocks however, self-sealing is expected to be a slower process. In specific, the kinetics of the self-sealing process in rocks in different states of induration may need further attention.
- The use of natural self-sealing should be more heavily exploited ("use of argillaceous host formations as their own natural analogues"). In many cases, arguments based on natural observations are more convincing than model calculations.

9.2.12 Stress regime

The stress regime is a FEP relevant for repository construction and operation (e.g. for repository layout, safety measures) as well as for PA (e.g. for gas migration, possible future faulting and flow along faults, EDZ evolution). Considerable problems exist in the experimental determination of the *in situ* stress state in argillaceous rocks. These constitute a material in which the standard stress measuring techniques, developed for hard rocks and for soils, are not easily applicable from both conceptual and technical points of view. An integrated approach with consideration of geological and technical stress indicators (e.g. borehole breakouts) and back-analyses (e.g. of convergence behaviour of tunnels in underground research laboratories) is commonly required for a consistent interpretation of *in situ* stress measurements.

9.3 Potential areas for future studies

On the basis of Section I, Chapters 7 and 8, a number of potentially promising actions emerged and are documented in Table 10. This table is not a comprehensive list of actions that addresses all open issues identified in the FEPs compilation (Section II), it is rather a list of potential actions that are considered promising and could result in major steps towards adequate understanding. The necessity to address the specific themes is variable among different sites due to different disposal concepts, requirements on the geosphere and regulatory demands.

Table 10. **Potential areas for future studies in argillaceous media**

Theme	**Objectives**	**Remarks**
Abnormal and normal pressures in the host formation	• Identification of underlying mechanisms (chemical osmosis, compaction disequilibrium, horizontal stress, erosion, ...) • Quantitative evaluation of all relevant mechanisms • Constraints on large-scale hydraulic conductivity and advective fluxes (upscaling in space) • Constraints for the expected long-term evolution (upscaling in time) • Comparative study integrating all available case studies in a uniform model framework (consistency check) • Evaluation of uncertainties (e.g. in the choice of initial and boundary conditions) • The model should explain both the presence of abnormal pressure at some sites and their absence at other sites	• Observed at several sites • Quantitative evaluation limited by uncertainties in head measurement and resulting hydraulic gradients • Details see Section I, Chapter 7.2.1
Natural tracer profiles across argillaceous formations	• Assessment of the relative importance of diffusion and advection as transport processes (e.g. constraints on vertical advective fluxes) • Constraints on large-scale diffusion coefficients (upscaling in space) • Constraints for the expected long-term evolution (upscaling in time) • Comparative study integrating all available case studies in a uniform model framework (consistency check) • Evaluation of uncertainties (e.g. in the choice of initial and boundary conditions) • The model should explain both the presence of spatial variability of tracer concentrations (or isotopic ratios) at some sites and its absence at other sites	• Suitable data available at several sites • Quantitative evaluation quite feasible due to high analytical precision and availability of several tracers in the same profile • Details see Section I, Chapter 7.2.2

Theme	Objectives	Remarks
Geochemical stability	• Evaluation of processes that may affect geochemical stability. • Evaluation of the buffering potential of the host rock against external geochemical perturbations. • Evaluation of the kinetics of the buffering reactions. • Comparative study integrating all available case studies in a uniform framework (consistency check). • Improve understanding of modelling bases for cation exchange reactions as controls on major ion chemistry.	• Details see Section I, Chapter 7.3
Understanding diffusion	• Improve understanding of diffusion of retarded species and cations by experimental work in laboratories and underground research laboratories. Sorption is important in establishing the rate of diffusive transport of retarded species, so understanding of both sorption and diffusion are important to interpret the results of such experiments. • Apply improved understanding of diffusion to evaluate formation geochemical stability and to develop and validate parameters used in support of PA.	• Details see Section I, Chapter 7.4
Understanding sorption	• Improve mechanistic understanding of sorption to enhance confidence in transport modelling results supporting PA. Such efforts are already being co-ordinated within the NEA Sorption Project.	• Details see Section I, Chapter 7.5
Time evolution and geometry of the EDZ, self-sealing	• Integrated view on types, distribution and development of fractures in the EDZ. • Evaluation of the commonalties and differences of EDZs in different argillaceous rocks in different degrees of induration. • Closure and self-sealing mechanisms of composite, wedge-shaped EDZ fracture planes in response to increased swelling pressure from the bentonite backfill. Large-scale and long-term experiments in underground rock laboratories may be employed for this purpose. • Improved quantitative understanding of processes underlying self-sealing.	• Still no unified theory on the characteristics of the EDZ. Wedge-shaped fracture planes may develop in the deeper parts of the EDZ. • Details see Section I, Chapter 7.6

Theme	Objectives	Remarks
Present-day stress regime	• Development of a systematic approach for the determination of *in situ* stress regimes in argillaceous rocks. Such an approach involves *in situ* stress measurements, geologic and technical stress indicators and backanalysis of the mechanical behaviour of the rocks around underground research laboratories. • Adjustment of the established *in situ* stress measuring techniques for argillaceous materials. • Systematic evaluation of the effects of the structural anisotropy (natural and induced) of argillaceous materials on the *in situ* stress measuring methods and on the *in situ* stress regime.	• Details see Section I, Chapter 7.7
Conceptual micro-mechanical models	• Awareness of the rapidly increasing potential of micro-mechanical modelling for a broad range of problems. • Identification and quantification of the mechanisms and processes at the micro-scale which can lead to “secondary creep”.	• Micro-mechanical models provide better insights into the relevant physico-chemical mechanisms than conventional generic models. • Details see Section I, Chapter 7.8
Effects of repository components on host rock and its pore-water chemistry (FEPs 28 and 30)	• The knowledge and awareness of this theme is very limited in some programmes. Only cement, steel and, to some extent, organics are considered in current designs. Future work should also consider the effects of soluble salts that may be present in some medium-level waste streams. The first step would be the compilation of an overall inventory of possible effects. • When systematic scoping work becomes available, the possibility exists that the relevance of this theme can be shown to be limited. • The results of the scoping work may serve to focus more detailed studies.	• Theme corresponds to FEPs 28 and 30 which are considered as relevant, while no general consensus on their understanding exists

Theme	Objectives	Remarks
Gas-induced transport in water	• Upscaling is the most difficult aspect of this theme. Existing uncertainty could be addressed by large-scale experiments in underground research laboratories.	• Theme corresponds to FEP 48 which is considered as relevant, while no general consensus on its understanding exists
Microbiological perturbations	• Substantial work is available for bentonite but not for the argillaceous host rocks. • The contention that microbes are not active in the matrix porosity due to space constraints could be substantiated by investigations in underground research laboratories (e.g. drilling with disinfected equipment). • The role of microbes in the EDZ could be addressed by 1) microbiological characterisation of fracture and matrix waters and 2) by studying water and gas chemistry and geochemical reactions catalysed by microbes.	• Theme corresponds to FEP 49 which is considered as relevant, while no general consensus on its understanding exists

9.4 The future of the FEPCAT project

The existing FEPCAT document is regarded useful (1) as a reference book reflecting current knowledge and (2) as a tool to guide future activities (both PA and R&D) in the field of geological disposal in argillaceous rocks. However, because major investigation programmes are ongoing both in the industrial and academic sectors, this document has a limited half life and further efforts are needed to keep the document up to date. The following activities might be suggested:

- *Recurrent updates of the compilation and the resulting conclusions.* This could happen when milestone reports from one of the participating organisations become available. Such updates would be performed on the basis of the new documents and on personal contacts. It is not envisaged to work on the basis of questionnaires.
- *Integration of results and conclusions of international topical conferences and workshops.* Attendance of such focussed meetings is regarded as an efficient method to update those FEPs which are covered by the theme of the conference/workshop.
- *Integration of the Clay Club Catalogue.* This data compilation, organised in an internally consistent format, is considered an ideal complement to FEPCAT, where the backgrounds and underlying processes are discussed, without focussing on numeric values. An updated version of the Catalogue will be published simultaneously with this report.
- *Actions emerging from feedbacks of the users of the FEPCAT report,* formally organised by the IGSC.

10. CORRELATION OF FEPs FROM THE FEPCAT PROJECT WITH THE NEA FEPs DATABASE

An international FEPs database has been developed under the auspices of the NEA and is documented in NEA (2000). The scope of this database is much wider than the one considered in FEPCAT. It is a generic database and thus not restricted to argillaceous rocks. Furthermore, it considers numerous features and processes that were screened out in FEPCAT, e.g. human actions, climate effects and waste characteristics. The level of detail, however, to which individual processes and characteristics are addressed in the FEPCAT project is higher compared to the NEA FEPs database. For example, there is just one FEP "Host rock", while numerous FEPs address the host rock in FEPCAT.

As indicated below, the structuring of the NEA FEPs database follows a different logic than the one used for FEPCAT. Together with the differing levels of detail of the two projects, this leads to the fact that in most cases there is no one-to-one correspondence of FEPs in the two databases. This is illustrated by the following examples:

- Several FEPCAT FEPs include aspects that belong to both NEA FEPs groups "Geological environment" *and* "Contaminant release/migration factors". This is because in FEPCAT, one FEP can address both the general characteristics of a FEP in an argillaceous formation as well as the consequences for radionuclide transport, while these aspects are separated in the NEA FEPs database. Thus each FEPCAT FEP may have more than one correspondence in the NEA FEPs database.
- The FEPs group "Geological environment" in the NEA FEPs database includes both natural and repository-induced effects, while these are separated in FEPCAT. Thus the NEA FEPs database makes no distinction between categories A and B of the FEPCAT FEPs database, thus several FEPCAT FEPs may relate to just one NEA FEP.

In general, it was found that the NEA FEPs database is comprehensive enough to accommodate most FEPCAT FEPs at logical positions. An exception are coupled thermo-hydro-mechanical processes which do not have a clear correspondence.

The NEA FEPs database is structured as follows:

0 Assessment basis
1 External factors
1.1 Repository issues
1.2 *Geological processes and effects*
1.3 Climatic processes and effects
1.4 Future human actions
1.5 Other
2. Disposal system domain: environmental factors
2.1 Wastes and engineered features
2.2 *Geological environment*

2.3 *Surface environment*
2.4 Human behaviour
3. Radionuclide/contaminant factors
3.1 Contaminant characteristics
3.2 *Contaminant release/migration factors*
3.3 Exposure factors

All FEPCAT FEPs relate to the four NEA FEPs groups that are printed in italics above, according to the limited scope of FEPCAT as described in Chapter I.1.2. Table 11 expands the NEA FEPs database structure given above by incorporating all those FEPs that are of concern for FEPCAT (in total 28 FEPs). A full integration of the FEPCAT FEPs list into the NEA FEPs database will be performed by NEA at a later stage.

Table 11. **Extract of the NEA FEPs database with FEPs that are of concern within the scope of the FEPCAT project**

0	**ASSESSMENT BASIS**
1	**EXTERNAL FACTORS**
1.1	REPOSITORY ISSUES
1.2	GEOLOGICAL PROCESSES AND EFFECTS
1.2.01	Tectonic movements and orogeny
1.2.02	Deformation, elastic, plastic or brittle
1.2.03	Seismicity
1.2.07	Erosion and sedimentation
1.2.08	Diagenesis
1.2.10	Hydrological/hydrogeological response to geological changes
1.3	CLIMATIC PROCESSES AND EFFECTS
1.4	FUTURE HUMAN ACTIONS
1.5	OTHER
2	**DISPOSAL SYSTEM DOMAIN: ENVIRONMENTAL FACTORS**
2.1	WASTES AND ENGINEERED FEATURES
2.2	GEOLOGICAL ENVIRONMENT
2.2.01	Excavation disturbed zone, host rock
2.2.02	Host rock
2.2.03	Geological units, other
2.2.04	Discontinuities, large scale (in geosphere)
2.2.05	Contaminant transport path characteristics (in geosphere)
2.2.06	Mechanical processes and conditions (in geosphere)
2.2.07	Hydraulic/hydrogeological processes and conditions (in geosphere)
2.2.08	Chemical/geochemical processes and conditions (in geosphere)
2.2.09	Biological/biochemical processes and conditions (in geosphere)
2.2.10	Thermal processes and conditions (in geosphere)
2.2.11	Gas sources and effects (in geosphere)
2.2.12	Undetected features (in geosphere)
2.3	SURFACE ENVIRONMENT
2.3.12	Erosion and deposition
2.4	HUMAN BEHAVIOUR

3	**RADIONUCLIDE/CONTAMINANT FACTORS**
3.1	CONTAMINANT CHARACTERISTICS
3.2	CONTAMINANT RELEASE/MIGRATION FACTORS
3.2.01	Dissolution, precipitation and crystallisation, contaminant
3.2.02	Speciation and solubility, contaminant
3.2.03	Sorption/desorption processes, contaminant
3.2.04	Colloids, contaminant interactions and transport with
3.2.05	Chemical/complexing agents, effects on contaminant speciation/transport
3.2.06	Microbial/biological/plant-mediated processes, contaminant
3.2.07	Water-mediated transport of contaminants
3.2.09	Gas-mediated transport of contaminants
3.2.11	Animal, plant and microbe mediated transport of contaminants
3.3	EXPOSURE FACTORS

An allocation of FEPCAT FEPs to the 28 FEPs of the NEA FEPs database is made in Table 12. The most commonly applicable FEPs from the NEA database are 2.2.02 (Host rock), 2.2.07 (Hydraulic/hydrogeological processes and conditions in geosphere) and 2.2.08 (Chemical/geochemical processes and conditions in geosphere).

Table 12. **Possible allocation of FEPCAT FEPs to FEPs from the NEA database**
n.a. = not available

FEPCAT FEPs database			**NEA FEPs database**	
FEP no. and hierarchy		**FEP name**	**FEP no.**	**FEP name**
	A	UNDISTURBED SYSTEM		
	A1	**Transport mechanisms**		
1	A1.1	Advection/dispersion	2.2.07 3.2.07	Hydraulic/hydrogeological processes and conditions (in geosphere) Water-mediated transport of contaminants
2	A1.1.1	*Size and geometry of the host rock and of surrounding units, migration path length*	2.2.02 2.2.03	Host rock Geological units, other
3	A1.1.2	*Migration pathways, including heterogeneity and anatomy*	2.2.04 2.2.05	Discontinuities, large scale (in geosphere) Contaminant transport path characteristics (in geosphere)
4	A1.1.3	*Undetected geological features*	2.2.12	Undetected features (in geosphere)
5	A1.1.4	*Hydraulic potentials and gradients in the host rock, including boundary conditions*	2.2.07	Hydraulic/hydrogeological processes and conditions (in geosphere)
6	A1.1.5	*Hydraulic properties of the host rock*	2.2.02 2.2.07	Host rock Hydraulic/hydrogeological processes and conditions (in geosphere)
7	A1.1.6	*Units over- and underlying the host formation: local and regional hydrogeologic framework*	2.2.03 2.2.07	Geological units, other Hydraulic/hydrogeological processes and conditions (in geosphere)

FEPCAT FEPs database			NEA FEPs database	
FEP no. and hierarchy		FEP name	FEP no.	FEP name
	A1.2	Diffusion		
8	A1.2.1	*Diffusivity*	2.2.02	Host rock
			2.2.08	Chemical/geochemical processes and conditions (in geosphere)
			3.2.07	Water-mediated transport of contaminants
9	A1.2.2	*Connected matrix porosity*	2.2.02	Host rock
10	A1.2.3	*Ion exclusion*	2.2.02	Host rock
			2.2.08	Chemical/geochemical processes and conditions (in geosphere)
11	A1.2.4	*Surface diffusion*	2.2.08	Chemical/geochemical processes and conditions (in geosphere)
			3.2.07	Water-mediated transport of contaminants
12	A1.3	Colloid formation, transport and filtration	3.2.04	Colloids, contaminant interactions and transport with
	A2	**Retardation mechanisms**		
	A2.1	Matrix diffusion		
8	A2.1.1	*Diffusivity*	2.2.02	Host rock
			2.2.08	Chemical/geochemical processes and conditions (in geosphere)
			3.2.07	Water-mediated transport of contaminants
9	A2.1.2	*Connected matrix porosity*	2.2.02	Host rock
13	A2.1.3	*Flow-wetted surface and accessibility of matrix*	2.2.05	Contaminant transport path characteristics (in geosphere)
10	A2.1.4	*Ion exclusion*	2.2.02	Host rock
			2.2.08	Chemical/geochemical processes and conditions (in geosphere)
11	A2.1.5	*Surface diffusion*	2.2.08	Chemical/geochemical processes and conditions (in geosphere)
			3.2.07	Water-mediated transport of contaminants
	A2.2	Sorption (broad definition)		
14	A2.2.1	*Lithology, mineralogy of rocks and fracture infills*	2.2.02	Host rock
			2.2.08	Chemical/geochemical processes and conditions (in geosphere)
15	A2.2.2	*Natural organics, complexation*	2.2.02	Host rock
			2.2.08	Chemical/geochemical processes and conditions (in geosphere)
			3.2.05	Chemical/complexing agents, effects on contaminant speciation/transport
16	A2.2.3	*Mineral-surface area*	2.2.02	Host rock
17	A2.2.4	*Pore- and fracture water composition*	2.2.08	Chemical/geochemical processes and conditions (in geosphere)
			3.2.02	Speciation and solubility, contaminant

FEPCAT FEPs database			NEA FEPs database	
FEP no. and hierarchy		FEP name	FEP no.	FEP name
18	A2.2.5	*Dissolution / precipitation of solid phases*	1.2.08 2.2.08 3.2.01	Diagenesis Chemical/geochemical processes and conditions (in geosphere) Dissolution, precipitation and crystallisation, contaminant
19	A2.2.6	*Solid solutions / co-precipitation*	3.2.01	Dissolution, precipitation and crystallisation, contaminant
20	A2.2.7	*Ion exchange*	2.2.08 3.2.03	Chemical/geochemical processes and conditions (in geosphere) Sorption/desorption processes, contaminant
21	A2.2.8	*Surface complexation*	2.2.08 3.2.03	Chemical/geochemical processes and conditions (in geosphere) Sorption/desorption processes, contaminant
22	A2.2.9	*Thermodynamic and kinetic modelling data*	2.2.08 3.2.01 3.2.02 3.2.03	Chemical/geochemical processes and conditions (in geosphere) Dissolution, precipitation and crystallisation, contaminant Speciation and solubility, contaminant Sorption/desorption processes, contaminant
	A3	**System understanding and independent methods / tools to build confidence in predictive models**		
23	A3.1	Palaeo-hydrogeology of the host formation and of embedding units	1.2.08 2.2.07	Diagenesis Hydraulic/hydrogeological processes and conditions (in geosphere)
24	A3.2	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units	1.2.08 2.2.08	Diagenesis Chemical/geochemical processes and conditions (in geosphere)
25	A3.3	Water residence times in the host formation	2.2.07 2.2.08	Hydraulic/hydrogeological processes and conditions (in geosphere) Chemical/geochemical processes and conditions (in geosphere)

FEPCAT FEPs database			**NEA FEPs database**	
FEP no. and hierarchy		**FEP name**	**FEP no.**	**FEP name**
	B	REPOSITORY-INDUCED PERTURBATIONS		
	B1	**Chemical perturbations**		
26	B1.1	Oxidation of the host rock	2.2.08	Chemical/geochemical processes and conditions (in geosphere)
27	B1.1.1	*Redox buffering capacity of the host rock*	2.2.02 2.2.08	Host rock Chemical/geochemical processes and conditions (in geosphere)
28	B1.2	Effects of repository components on pore-water chemistry in the host rock	2.2.08 3.2.02 3.2.05	Chemical/geochemical processes and conditions (in geosphere) Speciation and solubility, contaminant Chemical/complexing agents, effects on contaminant speciation/transport
29	B1.2.1	*Interactions of hyperalkaline fluids and host rock*	2.2.08 3.2.02 3.2.05	Chemical/geochemical processes and conditions (in geosphere) Speciation and solubility, contaminant Chemical/complexing agents, effects on contaminant speciation/transport
30	B1.2.2	*Organics from waste and their effect on transport properties of the host rock*	2.2.08 3.2.05	Chemical/geochemical processes and conditions (in geosphere) Chemical/complexing agents, effects on contaminant speciation/transport
	B2	**Thermal perturbations**		
31	B2.1	Thermal effects on mineral stability and pore-water composition	2.2.08 2.2.10	Chemical/geochemical processes and conditions (in geosphere) Thermal processes and conditions (in geosphere)
32	B2.2	Thermal rock properties	2.2.02 2.2.10	Host rock Thermal processes and conditions (in geosphere)
33	B2.3	Thermally induced consolidation of the host rock	n.a.	n.a.
	B3	**Geomechanical perturbations**		
34	B3.1	Geomechanical stability	2.2.06	Mechanical processes and conditions (in geosphere)
35	B3.2	Size and structure of the EDZ	2.2.01	Excavation disturbed zone, host rock
36	B3.3	Effects of bentonite swelling on the host rock	2.2.06	Mechanical processes and conditions (in geosphere)
37	B3.4	Geomechanical rock properties	2.2.02 2.2.06	Host rock Mechanical processes and conditions (in geosphere)

FEPCAT FEPs database			NEA FEPs database	
FEP no. and hierarchy		FEP name	FEP no.	FEP name
	B4	**Hydraulic perturbations**		
38	B4.1	Hydraulic properties of the EDZ	2.2.01 2.2.07	Excavation disturbed zone, host rock Hydraulic/hydrogeological processes and conditions (in geosphere)
39	B4.2	State of saturation of the EDZ and desiccation cracking	2.2.01 2.2.06	Excavation disturbed zone, host rock Mechanical processes and conditions (in geosphere)
	B5	**Perturbations from coupled processes**		
40	B5.1	Coupled thermo-hydro-mechanic processes	n.a.	n.a.
41	B5.2	Swelling	n.a.	n.a.
42	B5.3	Self-sealing	n.a.	n.a.
43	B5.4	Off-diagonal Onsager processes except chemical osmosis	n.a. in 2.2 3.2.07	n.a. Water-mediated transport of contaminants
44	B5.5	Chemical osmosis	2.2.08 3.2.07	Chemical/geochemical processes and conditions (in geosphere) Water-mediated transport of contaminants
	B6	**Perturbations from waste-derived gas**		
45	B6.1	Gas dissolution and chemical interactions between gas and pore-water	2.2.11	Gas sources and effects (in geosphere)
46	B6.2	Gas migration through the primary porosity (matrix, natural fractures)	2.2.11 3.2.09	Gas sources and effects (in geosphere) Gas-mediated transport of contaminants
47	B6.3	Gas migration through stress-induced porosity (gas fracs, pathway dilation)	2.2.11 3.2.09	Gas sources and effects (in geosphere) Gas-mediated transport of contaminants
48	B6.4	Gas-induced transport in water	2.2.11 3.2.07	Gas sources and effects (in geosphere) Water-mediated transport of contaminants
49	B7	**Microbiological perturbations**	2.2.09 3.2.06 3.2.11	Biological/biochemical processes and conditions (in geosphere) Microbial/biological/plant-mediated processes, contaminant Animal, plant and microbe mediated transport of contaminants

FEPCAT FEPs database			**NEA FEPs database**	
FEP no. and hierarchy		**FEP name**	**FEP no.**	**FEP name**
	C	LONG-TERM EVOLUTION		
	C1	**Diagenesis**		
	C1.1	Past basin evolution		
23	C1.1.1	*Palaeo-hydrogeology of the host formation and of the embedding units*	1.2.08 2.2.07	Diagenesis Hydraulic/hydrogeological processes and conditions (in geosphere)
24	C1.1.2	*Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units*	1.2.08 2.2.08	Diagenesis Chemical/geochemical processes and conditions (in geosphere)
50	C1.1.3	*Past burial history*	1.2.07 1.2.08 2.3.12	Erosion and sedimentation Diagenesis Erosion and deposition
	C1.2	Ongoing and future processes		
51	C1.2.1	*Present and future geothermal regime and related processes*	2.2.10	Thermal processes and conditions (in geosphere)
52	C1.2.2	*Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)*	2.2.08	Chemical/geochemical processes and conditions (in geosphere)
	C2	**Deformation events**		
53	C2.1	Past deformation events	1.2.01 1.2.02 1.2.03 2.2.04	Tectonic movements and orogeny Deformation, elastic, plastic or brittle Seismicity Discontinuities, large scale (in geosphere)
54	C2.2	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events	1.2.01 1.2.02 1.2.03 1.2.10 2.2.05 2.2.07	Tectonic movements and orogeny Deformation, elastic, plastic or brittle Seismicity Hydrological/hydrogeological response to geological changes Contaminant transport path characteristics (in geosphere) Hydraulic/hydrogeological processes and conditions (in geosphere)
41	C2.3	Swelling	n.a.	n.a.
42	C2.4	Self-sealing	n.a.	n.a.
55	C2.5	Present-day stress regime	2.2.06	Mechanical processes and conditions (in geosphere)
56	C2.6	Future stress regime	2.2.06	Mechanical processes and conditions (in geosphere)

FEPCAT FEPs database			NEA FEPs database	
FEP no. and hierarchy		FEP name	FEP no.	FEP name
	C3	**Erosion and burial**		
57	C3.1	Geomechanical effects of erosion/ unloading	1.2.02	Deformation, elastic, plastic or brittle
			1.2.07	Erosion and sedimentation
			2.2.06	Mechanical processes and conditions (in geosphere)
			2.3.12	Erosion and deposition
58	C3.2	Consolidation due to burial	1.2.02	Deformation, elastic, plastic or brittle
			1.2.07	Erosion and sedimentation
			2.2.06	Mechanical processes and conditions (in geosphere)
			2.3.12	Erosion and deposition
59	C3.3	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)	1.2.01	Tectonic movements and orogeny
			1.2.10	Hydrological/hydrogeological response to geological changes
			2.2.07	Hydraulic/hydrogeological processes and conditions (in geosphere)

SECTION II

FEPs Compilation

Section II of the report compiles and summarises the information provided by the participating organisations in the questionnaires and in interviews. Thus there is no rigorous ambition of completeness, even though the Expert Group attempted to include all key information. For each FEP, the compilation is structured as follows:

1. *Definition and generalities*: Defines the FEP and clarifies its scope. Definitions of terms are included where appropriate.
2. *Site-specific experimental information:* Both the types of investigation methods and the results and conclusions are addressed. In many cases, the relevant questionnaire information is organised in table format. Field data, laboratory experiments, *in situ* experiments in boreholes or underground research laboratories as well as modelling studies are included. If appropriate, information of generic type or relating to rock formations that are not addressed otherwise in this report may also be included (e.g. natural analogues, examples from the scientific literature).
3. *Scaling issues:* Addresses the spatial and temporal scales to which the experimental information is related and compares them with the scales required for PA. If needed, comments are made on the upscaling of experimental data and findings (in the broadest sense) to PA scales.
4. *Scientific level of understanding:* Provides a judgement on how well a FEP is understood qualitatively and quantitatively, irrespective of how it is used (or not used) in PA.
5. *Linked FEPs:* Provides a list of FEPs which are usfeul to *evaluate, understand, quantify and/or constrain the consequences* of the FEP under discussion. In contrast, the list does not refer to FEPs which the FEP under discussion *affects*. The choice of linked FEPs depends on several factors that are difficult to standardise or quantify (e.g. rock type, repository design, degree of linkage). Thus the list should not be over-interpreted and should be used only as a rough guidance. Due to the definition above, the total matrix of linkages is not symmetric. This means that FEP A may be linked to FEP B but not FEP B to FEP A. For example, FEP 33 (B2.3; Thermally induced consolidation of the host rock) is linked to FEP 50 (C1.1.3; Past burial history) because the latter is important to judge the extent to which the rock may consolidate in response to heat emitted from the waste. Here, one important question is "How much does the waste-derived thermal pulse exceed the temperature that the formation experienced during natural burial?". On the other hand, FEP 50 does not depend at all on repository effects such as the one dealt with in FEP 33.
6. *Level of understanding from a PA perspective and treatment in PA*: The requirements to understand a FEP for PA purposes are in many cases substantially more limited than those which would be desirable from an academic point of view. Some FEPs may be ignored or treated in a conservative way without having full scientific understanding. Empiric approaches (e.g. sorption K_ds) can in many cases shown to be sufficient for PA purposes, without having a detailed and quantifiable understanding of the underlying mechanistic principles.
7. *Available reviews:* Addresses reviews pertinent to specific sites, to the entire waste management community as well as to milestones in the scientific literature.
8. *Planned work:* Overview of planned activities that could be used to co-ordinate future efforts in specific fields.
9. *Overall evaluation:* Short summary of the key points of the compilation.

1. ADVECTION/DISPERSION (FEP A1.1)

1.1 Definition and generalities

Advection is a process in which dissolved species are transported by the flow of the solvent (i.e. ground water). In geological media, due to their heterogeneous structure, the rate of advection may vary considerably between transport paths. The resulting spreading of the dissolved species is termed (hydrodynamic) dispersion. When considering advection it is important to distinguish between advection-dominated and diffusion-dominated systems. If a formation is fractured and if the fractures are transmissive, then flow and transport rates through them usually dominate those of the matrix.

1.2 Site-specific experimental information

Formation/site	Type of information	Scale	Results and conclusions
Toarcian-Domerian at Tournemire	Measurement of hydraulic conductivity *in situ* and in the laboratory, natural tracer profiles	1-100 m	Very low hydraulic conductivity of the matrix (10^{-15} - 10^{-14} m/s) and of fractures (10^{-11} - 10^{-12} m/s) (Boisson *et al.*, 1997, 1998). Locally, fractures may be water-conducting and also discharge water into the tunnel. However, it is not evident that the fracture network is hydraulically connected on the scale of the formation. Tracer profiles in pore-water can be explained by diffusion as the dominant transport mechanism (Boisson *et al.*, 2001).
Spanish Reference Clay in a Tertiary basin	Hydraulic tests and head measurements in boreholes, observation of discontinuities	tens of m	Very low hydraulic conductivity (4×10^{-12} m/s) and small downward gradient (0.02) resulting in negligible advection; transport is diffusion dominated; discontinuities are no advective paths; advection is dominant in surrounding aquifers (Enresa, 1999).

Formation/site	Type of information	Scale	Results and conclusions
Opalinus Clay in the Zürcher Weinland and at Mont Terri	*In situ* and laboratory hydraulic and diffusion tests, interpretation of hydraulic-head distributions and tracer profiles	1 cm to 100 m	Hydraulic conductivity is very low (*ca.* 10^{-13} m/s) and is not influenced by presence of fractures (Gautschi, 2001); transport is diffusion dominated. Hydraulic overpressures in the Benken borehole and tracer profiles in pore-water at both locations (Gimmi, 2002, Pearson *et al.*, 2003, Nagra, 2002) also indicate the predominance of transport by diffusion even over larger spatial and temporal scales.
Boom Clay at Mol	*In situ* (underground research laboratory) and laboratory hydraulic and diffusion tests, head measurements and hydraulic tests in boreholes Determination of dispersion length from electromigration experiments with high flow rates	cm (*in situ* and laboratory) to tens of m (*in situ*), boreholes with regional spreading	Very low hydraulic conductivity (~2 x 10^{-12} m/s) and small downward gradient (0.02) resulting in negligible advection; transport is diffusion dominated; no indication of deviations from Darcy's law under high effective stress and gradients much larger than the natural gradient (Ondraf/Niras, 2002).
Boda Clay Formation at Mecsek	Hydraulic tests and head measurements in boreholes from the surface and from the exploratory tunnel	1 - 10 m	Fracture-dominated system, advection negligible in matrix.
Pierre Shale in south Dakota (Neuzil & Belitz, 1998)	Core and field measurements in boreholes from the surface	1 cm to tens of m	Hydraulic conductivities from core and borehole tests are 10^{-13} to 10^{-14} m/s.
	Modelling of heads in the underlying regional aquifer	several km	In Pierre Shale at depths > 1 km, regional vertical permeabilities are similar to core and borehole values. At shallower depths, they are from 10^{-9} to 10^{-11} m/s. This is attributed to vertically transmissive fractures that are open only at shallow depths and are separated horizontally by a km or more.

Formation/site	Type of information	Scale	Results and conclusions
Canadian argillaceous formations	Laboratory measurements, geophysical logging in boreholes	Laboratory data: 1-5 cm; synthetic studies: 10 m to 10 km	Katsube & Williamson (1998) studied a wide range of argillaceous formations in Canada (from unconsolidated, slightly compacted muds to indurated shales). Typical travel times are very long (0.03-30 m/Ma) and hydraulic conductivities are very low (10^{-15} to 10^{-11} m/s). In various cases, these results have been compared with geophysical logs.

In general, the studied argillaceous formations have a very low hydraulic conductivity and sometimes the natural hydraulic gradients are also small, resulting in diffusion-dominated transport and mostly negligible advection and hydrodynamic dispersion. Although discontinuities (fractures, fissures, etc.) may be present, in many cases their transport properties are similar to those of the matrix, and they do not act as advective pathways, namely in weakly and moderately consolidated formations. Conductivity measurements in the laboratory yield results comparable to those of *in situ* tests. Fracture flow plays a role in highly consolidated formations, such as the Palfris Formation at Wellenberg, the Boda Clay Formation and to some extent also in the Toarcian-Domerian at Tournemire. The measurement of hydraulic conductivities of 10^{-12} m/s or lower is difficult and lengthy.

1.3 Scaling issues

The low hydraulic conductivities of the studied argillaceous formations make direct measurements on the scale relevant for PA difficult (or even impossible). In underground research laboratories, measurements on a decametre scale are possible by measuring inflow rates into sealed sections and by measuring hydraulic gradients around the underground research laboratory. Upscaling to formation or basin level is in general done by combining and correlating results from different scales (laboratory and *in situ*), different locations and different techniques.

Profiles of tracers that occur in pore-waters of the argillaceous formation (e.g. ^{2}H, ^{18}O, Cl) often yield curved patterns that can be explained by diffusion (see FEP 24). At least in some cases, modelling of such profiles also places constraints on the maximum vertical advective fluxes (e.g. Gimmi, 2002 for the Opalinus Clay in the Zürcher Weinland). If hydraulic gradients can be constrained, such model calculations thus provide information on the large-scale (100 m and more) hydraulic conductivity.

1.4 Scientific level of understanding

Generally, advection in argillaceous formations is well understood and Darcy's law is reported to be valid. Indications for deviations from Darcy's law at gradients <1 exist from Opalinus Clay at Mont Terri and are reported in Nagra (2002). However, the collection of relevant measurements is difficult because of the very low flow rates. Data on hydrodynamic dispersion in the pore network are mostly lacking, but they are also not important due to the low flow rates.

1.5 Linked FEPs

FEP 2	Size and geometry of the host rock and of surrounding units, migration path length
FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 4	Undetected geological features
FEP 5	Hydraulic potentials and gradients in the host rock, including boundary conditions
FEP 6	Hydraulic properties of the host rock
FEP 7	Units over- and underlying the host formation: local and regional hydrogeologic framework
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 25	Water residence times in the host formation
FEP 41	Swelling
FEP 42	Self-sealing
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

1.6 Level of understanding from a PA perspective and treatment in PA

Where discontinuities do not behave as advective pathways, the level of understanding is in general sufficient from a PA perspective. In the case of systems where fracture flow dominates, care must be taken to obtain representative datasets for the rock volume in question, and to apply adequate techniques e.g. to identify fractures of all orientations.

In many PA studies concerning argillaceous formations, advection is explicitly treated in the PA calculations. The uncertainty related to the upscaling of hydraulic conductuvity values to PA scales is often addressed by parameter variations. Often this explicit treatment is done in the framework of *what if* calculations to demonstrate that advection is a negligible transport mechanism and that mass transport is dominated by diffusion. This explicit treatment also allows to determine under which conditions (e.g. gradients) advective transport starts to contribute significantly to the overall mass transport.

1.7 Available reviews

Horseman *et al.* (1996).

1.8 Planned work

None reported.

1.9 Overall evaluation

Advection/dispersion is an important transport process and is examined as part of all site investigations. In many cases, it is found that advective transport and hydrodynamic dispersion are negligible compared to diffusive transport. Only in cases where advective transport through discontinuities occurs could advection/dispersion be a dominant transport mechanism, and this is only the case in some highly consolidated formations.

2. SIZE AND GEOMETRY OF THE HOST ROCK AND OF SURROUNDING UNITS, PATH LENGTH (FEP A1.1.1)

2.1 Definition and generalities

PA-relevant characteristics of the system geometry include the depth, thickness and homogeneity of the host rock and the nature of the surrounding formations. The characterisation of host rock thickness and heterogeneity provides information on the advective or diffusive path length for contaminant release.

2.2 Site-specific experimental information

Formation/ site	Type of information	Results and conclusions
Callovo-Oxfordian at Bure	2D seismic survey (15 km^2), 3-D seismic survey (4 km^2, with seismic attributes), deep boreholes over *ca.* 10 km^2. Oil drillings, reprocessed seismics and surface outcrops considered in an area with a radius of 20-25 km around the underground research laboratory (under construction)	Flat-lying sedimentary sequence dipping 1-1.5° to NW. No faulting with vertical displacements >5 m observed within an area of 5 km around the underground research laboratory. Known faults (Gondrecourt, E; Marne, W) bound the investigation area. The thickness of the Callovo-Oxfordian varies between 130 m in the SE to 145 m in the NNW, and is 133 m at the site of the underground research laboratory. It is over- and underlain by limestone units. At the site of the underground research laboratory, its depth is between *ca.* 422 and 552 m. The *Marne fault* is located 20 km W of the underground research laboratory, has a NW-SE strike and dips to NE. It is a recurrently reactivated basement fault, and the vertical displacement of the Callovo-Oxfordian is 60 - 80 m. The *Gondrecourt graben* is located 5 km E of the underground research laboratory, strikes NE-SW and is *ca.* 1-2 km wide. Vertical displacement is *ca.* 60 m in the Jurassic. The Callovo-Oxfordian is directly over- and underlain by limestone units (Oxfordian and Middle Jurassic), which have aquifer properties near the surface but are less transmissive in the exploratory boreholes around the underground research laboratory site ($K < 3 \times 10^{-7}$ m/s, Babot 1999). Reference: Trouiller & Lebon (1999).

Formation/ site	Type of information	Results and conclusions
Toarcian-Domerian at Tournemire	110 year old, 2 km long railway tunnel through the formation, two new (1996), shorter tunnels with total length of 60 m, several boreholes	The Late Toarcian to Domerian is a flat-lying, *ca.* 200 m thick layer at 180-380 m below surface. The railway tunnel, which hosts the underground research laboratory, is situated in the upper part of the formation at a depth of *ca.* 230 m. The E-W-trending, subvertical *Cernon fault* juxtaposes Triassic to Early Jurassic formations with the Toarcian-Domerian at Tournemire some 800 m north of the laboratory site. Throw along this faults is >500 m, and the northern block was relatively uplifted. The *Cirque du Tournemire fault* is a NE-SW-trending branch of the Cernon fault and is located close to the southern entrance of the railway tunnel. The Toarcian-Domerian at Tournemire is directly overlain by the Aalenian limestone aquifer. Some 100 m of low-permeability marls of Domerian to middle Toarcian age separate the footwall of the argillaceous unit from the underlying Carixian limestone aquifer. Reference: Barbreau & Boisson (1994), Boisson *et al.* (1998).
Spanish Reference Clay in a Tertiary basin	7 seismic profiles (total length 130 km), 3 core drillings (in total >1 500 m core), older hydrocarbon drillings	In the study area within the Tertiary basin, the flat-lying argillaceous sequence of early Miocene age is 200-400 m thick and is buried under 140-280 m of younger sediments. The argillaceous formation is overlain by *ca.* 100 m of low-permeability marls, then by *ca.* 40 m of more permeable limestones and sandstones. Beneath lie 1 200-1 300 m of Paleogene limestones, sandstones and marls with higher permeabilities. The argillaceous formation contains numerous listric normal faults (most likely of syn-sedimentary origin). Steep faults cross cutting the whole formation were mapped on the basis of seismic profiles. The vertical throw of these faults is a few decametres at most. The reference depth of the repository is 100 m below the top of the host formation, i.e. in the upper third. The overlying marls are also included in PA calculations, even though with smaller K_d values.

Formation/ site	Type of information	Results and conclusions
Opalinus Clay at Mont Terri	Geometric definition of rock units based on • Surface mapping • boreholes drilled from the surface • 2 parallel tunnels + research laboratory tunnel • numerous boreholes drilled from the tunnels and from the research laboratory • balanced cross-sections	The underground research laboratory is located in an anticline of the Folded Jura Mountains. Folding occurred at 12-5 Ma b.p., and the area has been uplifting since 10 Ma. The thickness of Opalinus Clay is 160 m and includes an aberrant 5-10 m thick sandy-calcareous facies, which disappears towards E but becomes thicker towards W (Franche Comté). The depth range in the research laboratory is 230-320 m below surface. The *Main Fault* (>70 m long, occurs in 2 tunnels + research laboratory, *ca.* 1 m thick) is considered to be a relatively insignificant structure. 2D balanced cross-sections indicate that it possibly ends within the Opalinus Clay on its upper side; its bottom is most likely connected to a larger thrust. Sandy limestones (Early Dogger) in the hanging wall and marls (Late Liassic) in the footwall are local aquifers. References: Thury & Bossart (1999), Wermeille & Bossart (1999).

Formation/ site	**Type of information**	**Results and conclusions**
Opalinus Clay in the Zürcher Weinland	Geometry of host rock and surrounding units in an area of 50 km^2 based on an evaluation of a 3-D seismics survey (Birkhäuser *et al.* 2001) and a deep borehole (Benken, Nagra 2001)	The flat-lying sedimentary sequence dips *ca.* 5° to S. The host rock considered for waste disposal includes the Opalinus Clay and the overlying Murchisonae beds in Opalinus Clay facies. It is embedded within a sequence of confining units (in general low-permeability rocks including some local aquifers), which are considered as a secondary barrier for contaminant transport. The confining units are bounded by regional limestone aquifers at the top (Malm) and bottom (Muschelkalk). Good data quality and high spatial resolution of the 3-D seismics allow detailed analysis of geological structures on a metre scale (faults with a vertical displacement of at least 4 m have been documented in various seismic-attribute maps). Host-rock thickness is 100-120 m at a reference depth of 650 m. Upper confining units: Thickness *ca.* 100 m. Lower confining units: Thickness *ca.* 150 m. The seismostratigraphic evaluation of the 3-D seismics indicates the homogeneity of Opalinus Clay over the entire study area (no indications of strongly reflecting intercalations), and so the stratigraphic sequence encountered in the Benken borehole can be extrapolated laterally. There are only minor variations in the seismic attributes of the various formations of the confining units, i.e. there are no dramatic changes of the facies or the thickness of these formations. The main large structures are the “high zone of Benken” with its bounding elements of the ‘Rafz-Marthalen flexure’ in the south and the ‘Wildensbuch flexure’ in the north. Towards the E, the potential siting area is limited by the ‘Neuhausen fault’ (vertical displacement about 45 m). References: Nagra (2001, 2002), Birkhäuser *et al.* (2001).

Formation/ site	**Type of information**	**Results and conclusions**
Boom Clay at Mol	Geological maps, boreholes (cored & uncored), geophysical logging data, high-resolution seismic campaigns, studies in clay pits, trenches, underground research laboratory	The Boom Clay was deposited in the Campine Basin in the north-eastern part of Belgium. It dips gently (<1°) to NNE and is characterised by a high lateral continuity. It crops out in the southern part of the Campine Basin and reaches a depth of about 400 m in the north. In the Roer Valley Graben in the outmost NE part of the Campine Basin, the Boom Clay is present at a far greater depth. In the vicinity of Mol, the clay formation is about 100 m thick. It is sandwiched between more permeable, sandy formations. The Boom Clay was investigated by several seismic campaigns on a regional scale (2D-seismic campaign PLM 1984 by the Geol. Survey of Belgium), and on a local scale: 3-D-seismic campaign 78-ON in the nuclear zone of Mol/Dessel (1978), a test line in 1991 (91-ON) and 65 km of high-resolution 2D-seismics covering an area of 15 km by 15 km around and inside the nuclear zone (96-ON). Three boreholes were drilled in the nuclear zone of Mol/Dessel: Dessel-1 (1993) and the cored boreholes SCK-15 (1975) and Mol-1 (1997). . References: Demyttenaere & Laga (1988), Wouters & Vandenberghe (1994).
Yper Clay at Doel	Geological maps, boreholes, studies in clay pits, offshore and canal seismic investigations	The Ypresian Clays were deposited in the northern and western part of Belgium. They dip gently (<1°) to NNE, reaching a thickness of 150 m, and occur at a depth of more than 600 m on the northern Belgian border. Their vertical and horizontal continuity is more variable when compared to Boom Clay. The Ypresian clays are composed of 4 members, characterised by a different lithologies (some are silty), and tend to become more sandy to the east. So the Moen Clay disappears to the east of Antwerpen, where it is known as the Mons-en-Pévèle Sand. Reference: LTGH-University Gent (1996).

Formation/ site	Type of information	Results and conclusions
Boda Clay Formation at Mecsek	45 boreholes from the surface down to max. 2 000 m (total length 5 300 m), 346 m long tunnel (underground research laboratory, Alfa tunnel system at 1 030-1 080 m depth), 70 boreholes from the tunnel (total length 2 300 m), surface mapping of outcrops	Known occurrence of the Boda Clay Formation is over 150 km^2. The size of the area suited for waste disposal is *ca.* 60 km^2 and located in the central part of the Western Mecsek anticline where the formation is 700-1 000 m thick. Internal structure: • Lower 150 m: Dominated by silt- and sandstones • Central part: 350-450 m thick argillaceous sequence with sandstone and siltstone beds • Upper part: 400-500 m thick argillaceous sequence with dolomitic beds. This unit hosts the underground research laboratory. It consists of cycles of reddish brown, silty, albitic shale beds and thin layers alternating with dolomite interbeddings with desiccation cracks and also contains dolomite concretions. Overlying unit: Fractured sandstones with U deposits (focus of past mining activities). Underlying unit: Fractured sandstone. A 80 m wide subvertical fault zone was penetrated by the tunnel and has a vertical displacement of 350-400 m. A large number of smaller fault hierarchies was also penetrated.
Mizunami Group at Tono	Field mapping and boreholes in the Tono area, underground research laboratory	Miocene argillaceous sequences include the Toki Lignite-bearing Formation (non-marine; basal conglomerate, sandstone and mudstone; 80 to 170 m in thickness), the Akeyo Formation (marine; mudstone and tuffaceous sandstone; 30 to 50 m in thickness), the Oidawara Formation (marine; basal conglomerate and massive mudstone; 40 to 45 m in thickness). They are cut by the Tsukiyoshi fault with vertical reverse displacement about 30 m in the Tono mine (Yusa *et al.*, 1992, Yoshida *et al.*, 1995).

Most sites characterised above are situated in large sedimentary basins, and the target formations are largely flat-lying. The surrounding formations are either regional aquifers or formations containing more permeable beds that have a more limited isolation capacity. Exceptions are the Mont Terri underground research laboratory in Opalinus Clay and, not presented above, the Wellenberg Site in the Central Swiss Alps. These sites are located in mountain chains and underwent major internal deformation.

2.3 Scaling issues

Field information relates to the same scales as those needed in PA.

2.4 Scientific level of understanding

Knowledge of the large-scale geometry is, in general, sufficiently well understood for both scientific and PA purposes.

2.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 4	Undetected geological features
FEP 7	Units over- and underlying the host formation: local and regional hydrogeologic framework
FEP 50	Past burial history
FEP 53	Past deformation events
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

2.6 Level of understanding from a PA perspective and treatment in PA

In host formations in which fracture flow is of low relevance, some transport-relevant parameters (such as diffusion coefficients and hydraulic conductivities) are anisotropic, with higher values parallel to bedding (i.e. in subhorizontal directions). Transport through such formations will occur laterally to some degree, thus the transport path lengths are expected to be longer when compared to the most direct route out of the formation. Nevertheless, for PA purposes, the most conservative assumption is made by assuming vertical upward transport. Discontinuities such as faults may be included explicitly in PA calculations. This is mostly done in alternative or *"what-if"* cases because such discontinuities have either not been identified in the target areas or have been shown to have no relevance for flow and transport (see FEP 3).

For formations where fracture flow is important, transport through them may be modelled explicitly. Alternatively, fluid flow can be simulated using an equivalent porous medium approach with average hydraulic conductivities higher than those of the matrix itself. Simulating transport with an equivalent porous medium model is done using very low flow porosities which lead to the high transport rates typical of flow in fractures.

The role of the surrounding units in PA is mostly limited to dilution. In some cases, surrounding units are included explicitly in PA calculations but in a simplified way (e.g. homogeneous layers). In other cases, they are ignored for the sake of conservatism; i.e. radionuclides released from the host formation are thought to be instantaneously transported into the regional aquifers.

2.7 Available reviews

Formation site	Reference
Callovo-Oxfordian at Bure	Andra (1999a) CNRS & Andra (1999)
Toarcian-Domerian at Tournemire	Barbreau & Boisson (1994), Boisson *et al.* (1998)
Opalinus Clay at Mont Terri	Thury & Bossart (1999)
Opalinus Clay in the Zürcher Weinland	Nagra (2001), Nagra (2002)
Boom Clay at Mol	Wouters & Vandenberghe (1994)
Boda Clay Formation at Mecsek	Hamos *et al.* (1996)

2.8 Planned work

None reported.

2.9 Overall evaluation

The thickness and depth location of the host rock are important parameters in PA. Present-day knowledge can be considered sufficient in most cases.

3. MIGRATION PATHWAYS, INCLUDING HETEROGENEITY AND ANATOMY (FEP A1.1.2)

3.1 Definition and generalities

Migration pathways (or water-conducting features) are zones with enhanced transmissivities within a rock body (Doe, 1999). If they are interconnected on a large scale and hydraulic gradients exist, advection and advective transport occur. Water-conducting features can be of sedimentary origin (lithologic heterogeneities, such as calcareous or sandy beds) or of tectonic origin (e.g. faults, joints). They are inherently spatially heterogeneous in both structure and hydraulic properties. They can be classified by origin, geometry and/or size. Relevant attributes are: Fracture aperture, flow (effective) porosity, flow-wetted surface, rock domains (e.g. fracture fillings, wall-rock domains/lithologies).

Faults or joints occur mainly in indurated argillaceous formations (e.g. Bjørlykke, 1994, Bjørlykke & Høeg, 1997). Typically, only a fraction of all the faults and joints in the rocks is hydraulically active, whereas others are sealed. Self-sealing of fractures that may exist is very efficient in soft clays, such that faults and joints are generally hydraulically irrelevant (see FEP 42). Water-conducting features of sedimentary origin (e.g. limestone beds) may occur in all types of argillaceous media.

3.2 Site-specific experimental information

Formation/ site	Type of information	Results and conclusions
Toarcian-Domerian at Tournemire	Surface mapping, tunnel wall and borehole logging, interpolation between boreholes, geophysical methods	Evidence based on boreholes and tunnel outcrops indicates that the rocks are fractured. However, transmissivity is very low in most fractures and faults, with a few exceptions where flow occurs at least locally. The larger-scale connectivity of the fracture network (in terms of geometry and hydraulics) is not well known.
Spanish Reference Clay in a Tertiary basin	Seismic surveys	Seismic surveys indicate the presence of subvertical discontinuities exclusively in a 1 km wide band of the Spanish Reference Clay. They are considered to be of non-tectonic origin (decompaction and/or dehydration structures). Otherwise, the formation is considered to be free of heterogeneities. Fracture flow is not considered in PA calculations.

Formation/ site	Type of information	Results and conclusions
Opalinus Clay at Mont Terri	Observations and measurements in tunnels and boreholes	Laboratory tunnel: Apart from minor but ubiquitous fracturing, a thrust fault (thickness 1 m, length >70 m) is intersected by 3 tunnels, without any water inflows or moisture zones (Thury & Bossart 1999). A borehole was drilled through this fault, and a hydraulic testing campaign was conducted. The conclusion was that the hydraulic properties of the fault cannot be distinguished from those of the rock matrix outside the fault. It follows that self-sealing processes were (and still are) very efficient in sealing major faults at this site. Mineralisations in the fault are virtually absent, indicating that water flow has also been limited throughout geological evolution. Motorway and safety tunnel: 2 drip points were observed in sandy-calcareous beds of Opalinus Clay at a depth of 150-200 m below surface (Gautschi 2001). It is remarkable that in spite of complex thrust tectonics, the formation does not yield any water to the tunnels at overburden depths >200 m.
Opalinus Clay in northern Switzerland	Observations in boreholes, in core materials, tunnels and quarries	Benken borehole (Nagra 2001): Only few natural fractures were observed over the 95 m long profile across the Opalinus Clay. None of these fractures has a hydraulic signature (nor do sandy beds). The whole profile shows superhydrostatic pressures, indicating very low permeability on a large scale. Opalinus Clay in quarries of northern Switzerland: Steeply dipping fracturing occurs, and the fractures are considered to be surface-related decompaction joints. In the uppermost 20-40 m, these joints have oxidised alteration rims, indicating water-rock interaction with meteoric water (Mazurek *et al.* 1996). No positive evidence of such interaction was found at deeper levels. Only few faults were observed (thickness max. 1 m, length up to tens of m) and are invariably filled by fault gouge (Nagra 2002). Opalinus Clay in boreholes from southern Germany: Hekel (1994) measured Cl contents in aqueous leachates from drillcore samples and identified a depleted zone in the uppermost 25 m below surface. Below this level, Cl contents are around 10 g/l and constant with depth, indicating that surface effects penetrated only to depths of 25 m. Opalinus Clay in railway tunnels in the Jura Mountains: A total tunnel length of *ca.* 6 000 m cross cuts the Opalinus Clay, and over this distance only 3 moisture zones were observed (Gautschi, 2001). All of these occur in shallow regions with less than 200 m overburden.

Formation/ site	**Type of information**	**Results and conclusions**
Boom Clay at Mol	Observations in the second shaft of the Mol underground research laboratory, in boreholes (incl. geophysical logs) and in clay pits. High-resolution seismics in the Mol area.	In the underground research laboratory at Mol, m-long slickensides and septaria (carbonate nodules) were identified as structural heterogeneities. The former are most likely artifacts of tunnel construction and thus part of the excavation-disturbed zone. A possible indication for preferential migration paths was observed in a radiochemical study which indicated that uranium and radium isotopes have been mobilised in the “Double Band”, which is the most silty layer of the Boom Clay (De Craen *et al.*, 1999, 2000). Although the formation is characterised by an alternation of more clayey and silty layers, it can be regarded as homogeneous and is devoid of discrete features that could lead to migration of radionuclides to the aquifers. Joints are present in outcrops but not in the underground research laboratory. Faults with visible displacement are observed in one quarry only. The identification of natural shear planes in the underground research laboratory is complicated by the large disturbance related to excavation (EDZ).
Yper Clay at Doel	Observations in clay pits, offshore seismics	Identification of intraformational faults with a thrust ranging from some decimetres to 3 metres (Henriet *et al.*, 1990).
Boda Clay Formation at Mecsek		The formation is highly consolidated and contains a fracture network that is composed of different sets of fracture families: 1. Regional E-W-trending, steeply dipping faults are the result of Cretaceous compression and have vertical throws of up to several 100 m. They are invariably filled by fault gouge and breccia, and their hydraulic conductivity is therefore limited (10^{-10} m/s were measured in boreholes across such faults). 2. NW-trending, steeply dipping joints are mostly sealed by calcite veins and therefore have a limited hydraulic conductivity over larger scales. 3. ENE-WSW-trending shear fractures of Paleogene-Miocene age contain mostly chloritic infills. They are hydraulically active today. 4. A second subvertical, NW-striking fracture system contains infills rich in clay minerals and partially reactivates the calcite vein-systems. It is locally water-conducting. 5. Bedding-parallel shear planes along sedimentary discontinuities (due to the anticlinal deformation) may also conduct water. In the laboratory, tracer migration tests through intact and microfractured cores were conducted. The two types of samples yield very similar breakthrough curves, which means that transport through microfractures is less important than through the porous matrix.

3.3 Scaling issues

Small-scale heterogeneities down to a few centimetres can be detected in outcrops, on tunnel walls and in cores, larger ones (>10 cm) in wireline logs. Faults with vertical throws larger than a few metres are visible in high-quality seismic profiles. However, the large-scale hydraulic characteristics of such water-conducting features are difficult to study, unless they were penetrated by boreholes or tunnels. In general, major features, if present, are avoided in most repository designs, thus no detailed characterisation is required from a PA viewpoint.

If only vertical boreholes are available, steeply dipping discontinuities may not be detected. If vertical displacements along them are small, they will also not be identified by seismic tools. Surface outcrops, e.g. in clay pits, are suited to fill this gap. A robust characterisation becomes available in the later stages of a site characterisation project, i.e. when a underground laboratory is built.

The large-scale hydraulic characteristics of discrete discontinuities, whether observed directly or not, can in many cases be constrained by the quantitative interpretation of head profiles (hydraulic disequilibria, i.e. under- or overpressures) and profiles of geochemical tracers, such as He, Cl, ^{37}Cl, ^{18}O and ^{2}H in pore-water (see FEP 24).

3.4 Scientific level of understanding

In general, sedimentary heterogeneities are well understood. With respect to the understanding of tectonic structures on different scales and their significance for migration, the spectrum of judgements is heterogeneous. One of the main difficulties is the upscaling of geological and hydraulic observations made on small scales (boreholes, tunnels) to PA-relevant scales (see above).

3.5 Linked FEPs

FEP 4	Undetected geological features
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 18	Dissolution/precipitation of solid phases
FEP 41	Swelling
FEP 42	Self-sealing
FEP 53	Past deformation events
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

3.6 Level of understanding from a PA perspective and treatment in PA

At all considered sites, sedimentary heterogeneities are regarded as well understood and not critical to PA. On the other hand, the explorability and PA significance of tectonic features is a matter of debate in the case of indurated (often over-consolidated) formations, less so in the case of plastic clays. Some good indications exist that faults are hydraulically insignificant in argillaceous formations. However, in some cases the data base is limited, such that it is difficult to rigorously demonstrate the irrelevance of tectonic structures for flow and transport.

Other open questions include:

1. Spatial heterogeneity and large-scale anatomy of tectonic water-conducting features, namely faults, and their conceptualisation;
2. Scaling rules of faults;
3. Relevance of episodic deformation and flow events (FEP 54).

The PA approaches are fundamentally different for soft and fractured clay formations:

- Soft clays, such as the Boom Clay and the Spanish Reference Clay, are considered to be diffusion-dominated, with a negligible contribution of fracture flow. The diffusion-dispersion model is applied for PA calculations. Known fractured zones, whether hydraulically active or not (e.g. in the Spanish Reference Clay), are avoided by repository design.

- Indurated clay formations, such as the Boda Clay Formation, are assumed to be dominated by fracture flow, and thus a double-porosity approach is used.

- Formations in an intermediate stage of induration are the Opalinus Clay and the Callovo-Oxfordian at Bure. While evidence exists that these formations are diffusion-dominated (hydraulic evidence, natural tracer profiles), (over)conservative assumptions about the existence of long, interconnected, water-conducting fractures can be explored in alternative or *what-if* model calculations of radionuclide transport.

3.7 Available reviews

Formation/site	Reference
Generic	NEA (1998a,b)
Callovo-Oxfordian at Bure	Andra (1999a)
Toarcian-Domerian at Tournemire	Boisson *et al.* (1998), Cabrera (2001)
Opalinus Clay at Mont Terri	Thury & Bossart (1999)
Opalinus Clay in the Zürcher Weinland	Nagra (2001), Nagra (2002)
Boom Clay at Mol	Wouters & Vandenberghe (1994)
Boda Clay Formation at Mecsek	Hamos *et al.* (1996)

3.8 Planned work

Boom Clay at Mol: Analysis of large-scale heterogeneities (e.g. slickensides, joints) in outcrops and in the underground research laboratory. Special processing of available seismics.

3.9 Overall evaluation

The understanding of tectonic migration pathways, including their geometry and hydraulic significance, is generally regarded as moderate to very good, depending on the degree of detail of the site investigations. Apart from further structural characterisation, indirect evidence (e.g. palaeo-hydrogeological arguments, environmental tracers) may help to understand transport through the formations. Fracture flow is unlikely in soft clays but may dominate transport in highly indurated argillaceous formations.

4. UNDETECTED GEOLOGICAL FEATURES (FEP A1.1.3)

4.1 Definition and generalities

This FEP relates to features that cannot currently be observed because of the lack of appropriate techniques, or features that were not detected yet because of insufficient studies.

4.2 Site-specific experimental information

Sedimentary heterogeneities, such as lateral changes in facies, are expected to occur on a regional scale and are generally well constrained by information from boreholes and surface outcrops. They are not regarded as sources of major uncertainty. The situation is less clear for tectonic heterogeneities. Faults in seismic surveys are only recognised if their vertical throw at the bottom and/or top of the target formation exceeds 5-10 m. If the faulting mechanism was dominated by strike-slip, even major faults may stay undetected prior to drilling or tunnelling activities. In highly indurated argillaceous formations, such faults may play a role as migration pathways. However, they do not disrupt the lateral continuity of the formation whose thickness is at least one order of magnitude larger than the seismic detection limit. At least in the case of the Opalinus Clay of the Zürcher Weinland, all faults mapped on the surface have a vertical component of displacement, i.e. pure strike-slip faults were not observed.

In the national programmes aimed at the characterisation of disposal sites or underground research laboratories, no example exists where the initial conceptual model of the site had to be changed substantially due to the later discovery of new features.

Indirect evidence suggesting the existence of undetected features is documented in the Pierre Shale (North America). In this formation, different in situ methods were used to measure hydraulic conductivity, resulting in values of 10^{-14}-10^{-13} m/s (Neuzil, 1986, 1993). In contrast, regional simulations of a system of multiple aquifers and confining units in south Dakota yields values of 10-9 m/s, i.e. 4-5 orders of magnitude higher than the local ones (Bredehoeft *et al.*, 1983). This disparity is interpreted as an effect of large-scale, conductive features (faults, fractures, clastic dykes), which, in spite of an extensive drilling programme, could not be detected directly. For other basins where the Pierre Shale or its equivalents occur (Denver and Alberta basins), the regional and local conductivities are consistently low, i.e. there is no indication of the presence of undetected features. The following references are relevant for this case study, sorted after spatial scale:

Laboratory/core scale:	Neuzil (1986), Bredehoeft *et al.* (1983)
Borehole scale:	Neuzil (1993), Bredehoeft *et al.* (1983)
Kilometre scale:	Neuzil (1993)
10^2 kilometre scale:	Bredehoeft *et al.* (1983), Belitz & Bredehoeft (1988), Corbet & Bethke (1992), Neuzil (1995a, b)
Continental scale (>10^3 km):	Neuzil (1995a, b).

4.3 Scaling issues

The question of possibly undetected features originates in the fact that the scale of observation is smaller than the total volume of rock of interest. While seismic methods relate to large scales, their spatial resolution is limited.

4.4 Scientific level of understanding

Limitations in explorability of currently used methods are the main source of uncertainty. It can be reduced by combining information and understanding obtained at different scales (regional geological studies, boreholes, geophysical techniques). Moreover, uncertainty will decrease during each step of site characterisation, so it is also a function of the maturity of the project.

As an example, the nature, density and disposition of transmissive features in the Pierre Shale remains poorly understood. Their apparent presence in only certain areas may be a result of stress (and therefore depth) dependence; the base of the shale is shallower (<1 km) in south Dakota than in either the Denver or Alberta Basins.

A counter-example is the Opalinus Clay in northern Switzerland, where both environmental tracers in pore-water as well as hydraulic overpressures indicate that permeability is very low over large scales in space and time, which is consistent with measurements *in situ* and in the laboratory.

4.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 53	Past deformation events
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

4.6 Level of understanding from a PA perspective and treatment in PA

Lateral sedimentary heterogeneities are generally regarded as sufficiently well known. In some host formations, in specific in units that are not highly consolidated, faults have been shown to be hydraulically irrelevant, thus their detection is not of crucial importance from a PA perspective. The situation may be different for indurated shales where fracture flow may occur. In such cases, high-resolution seismic techniques (e.g. analysis of seismic attributes in 3-D surveys) and consideration of independent geochemical information (environmental tracers, ground-water ages) reduce uncertainty.

The existing uncertainty is accounted for in some PAs by minimising the path length from the repository to the surrounding rock units to the shortest distance possible, i.e. assuming a vertical upward migration path. For this case, it is very unlikely that major features could have been missed in the repository-tunnel system. In other PAs, transmissive features are explicitly included at least in alternative scenarios, in order to assess the consequences.

4.7 Available reviews

None reported.

4.8 Planned work

None reported.

4.9 Overall evaluation

Undetected features are issues in some but not all argillaceous systems and siting programmes. In PA, existing uncertainty is covered by conservative assumptions. Uncertainty can be reduced by high-resolution 3-D seismics, and it will also decrease with each phase of site investigations (e.g. when oblique boreholes are drilled or tunnels are built).

5. HYDRAULIC POTENTIALS AND GRADIENTS IN THE HOST ROCK, INCLUDING BOUNDARY CONDITIONS (FEP A1.1.4)

5.1 Definition and generalities

This FEP refers to the driving forces for (Darcy) fluid flow. Flow can also be driven by other forces (see Section II, Chapter 5.5).

5.2 Site-specific experimental information

Formation/ site	Type of information	Scale	Results and conclusions
Callovo-Oxfordian at Bure	Hydraulic tests, long-term monitoring	scale of the thickness of the formation (*ca.* 100 m)	Hydraulic overpressures of several tens of metres relative to the over- and underlying aquifers were identified in several boreholes (Andra 1999a). The overpressures are regarded as a real phenomenon, either due to 1) the consolidation of the formation during burial; or to 2) osmotic pressures (Andra, 1999a).
Toarcian-Domerian at Tournemire	*In situ* measurements from the underground research laboratory with different tools	Measurements distributed over range of several 100 m	Hydraulic heads show a quasi-linear trend between the values of the over- and underlying aquifers. Thus the boundary conditions determine the head distribution, and no anomalies are observed (Boisson *et al.*, 1997, 1998, 2001). Uncertainties include technical difficulties of pressure measurement, H-M-C coupling and the possible influence of 110 year old tunnel. Comparison with numerical model yields acceptable differences.

Formation/ site	Type of information	Scale	Results and conclusions
Spanish Reference Clay in a Tertiary basin	Continuous multi-level pressure measurement in deep borehole (4 in the argillaceous unit, 2 in overlying aquifer); geological model of sedimentary basin	Single deep borehole; basin size 1 300 km^2	Indications of a downward gradient (0.1-0.2 m/m, Enresa, 1999, Lopez Geta *et al.*, 1995). No abnormal pressures observed.
Opalinus Clay in the Zürcher Weinland	One deep borehole with several packer tests and long-term monitoring system	Single deep borehole	Slight overpressures observed in packer tests in Opalinus Clay and some underlying units. The long-term monitoring system does not record these overpressures, possibly for methodological reasons (short circuits). The overpressures are thought to be real phenomena and are explained as remnants of maximum burial and compaction that occurred *ca.* 10 Ma b.p. and/or horizontal stresses and strains related to the compressive tectonic regime (Nagra, 2002).
Opalinus Clay at Mont Terri	Measurements in boreholes drilled from tunnel (13 locations)	dm	No indication of abnormal pressures. Strong influence of the tunnel to at least 20 m distance (decompression). Hydraulic boundary conditions (adjacent aquifers) are not well characterised (Thury & Bossart, 1999).
Boom Clay at Mol	Several tens of piezometres installed from HADES underground research laboratory with measurements over more than 15 years	cm	No indication of abnormal pressures, downward gradient over Boom Clay (0.02 m/m). Influence of the tunnel up to 20 m distance (mainly drainage). Limited knowledge about the permeability and the heads in the underlying aquifers precludes full understanding of the field and laboratory observations (Ondraf/Niras, 2002).
	Hydraulic boundary conditions: piezometry of over- and underlying aquifers from (deep) boreholes (20 years)	Local and regional	
	Hydrogeological modelling	Local and regional	

Formation/ site	Type of information	Scale	Results and conclusions
Yper Clay at Doel	4 boreholes with filters in surrounding aquifers		Upward hydraulic gradient of about 0.2 m/m, no pressure measurements in the clay itself (Ondraf/Niras, 2002).
Boda Clay Formation at Mecsek	• 4 boreholes in Western Mecsek region • Several long-term multi-packer systems in boreholes (up to 160 m deep) in exploratory tunnel • Large-scale (regional) 3-D hydraulic model and hydro-mechanical model of tunnel surroundings	100 m to regional	No indication for over- or underpressures. Clear indication of drainage to the tunnel (Ormai *et al.*, 1996).
Pierre Shale in south Dakota	• Long-term measurements in deep boreholes at several levels (sealed-in instruments) • Hydraulic model of the Hayes region	km	Indication of strong underpressures (Neuzil, 1993).

Hydraulic pressure measurements in generally very low-permeability argillaceous rocks are difficult and require well adapted equipment and very careful installation. Important factors here are: the quality of the sealing and the dead volume in the measurement sections, the stiffness of the equipment, the chemistry of the test fluid, and the stability of the borehole wall and measurement sections. It is clear that these measurements are often more difficult in indurated shales than in plastic clays because of the lower hydraulic conductivity of the indurated shale and the more limited creep that can help to seal the test sections. In general, observations have required very long equilibration times (months to several years) so that long-term measurements are needed to obtain reliable data. These technical difficulties apply to measurements both in deep boreholes from the surface and in short drillings from tunnels.

Measurements from underground research laboratories or tunnels are influenced by the presence of the tunnel up to tens of metres from the tunnel walls, i.e. well beyond the EDZ. This can either be a purely hydraulic effect (drainage to the tunnel) or a coupled hydro-mechanical effect (see below).

Measurements of the heads in the surrounding aquifers are needed to allow an interpretation of the observed heads in the argillaceous formation.

In several cases over- or underpressures have been observed with respect to the heads expected based on the hydraulic boundaries. These could often be explained as consequences of relatively fast (geologically speaking) subsidence or uplift-erosion phenomena, by horizontal strains or, at least in some cases, by osmotic potentials. It has been demonstrated experimentally that anomalous pressures can be produced in boreholes by osmosis between borehole and formation fluids (see FEP 44).

5.3 Scaling issues

When deep aquifers are considered, the field observations of the hydraulic heads need to be made at the scale that one needs in the hydrogeological model (e.g. local, regional). This requires extended piezometric networks and thus a large number of drillings especially for regional scale models.

5.4 Scientific level of understanding

At sites where the hydraulic boundary conditions and the burial/deformation history are known and where sufficiently reliable measurements are available, the level of understanding of the hydraulic potentials is high. In several cases, the measured stable potentials can be explained by hydrogeological modelling (or coupled hydro-mechanical modelling) both in qualitative and quantitative terms (e.g. Ondraf/Niras, 2002, Nagra, 2002).

At sites where only measurements from tunnels are available and where the boundary conditions are unknown or less clear due to the presence of water-conducting features, the understanding of the hydraulic potentials is generally less good. When the effect of the tunnel is only drainage, this is well understood and can be successfully included in models. However, when the tunnel induces a coupled hydro-mechanical influence, the quantification is much more difficult.

The transient measured during the equilibration time of the measurements is commonly not well understood (nor modelled), probably because several coupled processes are acting at the same time.

The understanding of the processes underlying abnormal formation pressures is limited. While a number of processes can be invoked, their quantification is difficult because relevant parameters are not all well known (e.g. large-scale hydraulic conductivity and its dependence on hydraulic gradient, osmotic efficiency). The most frequently quoted processes to explain abnormal pressures are hydro-mechanical coupling (e.g. compaction due to increased overburden, decompaction due to erosion or melting of glaciers) and geochemical coupling (osmosis).

5.5 Linked FEPs

FEP 7	Units over- and underlying the host formation: local and regional hydrogeologic framework
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 40	Coupled thermo-hydro-mechanic processes

FEP 43 Off-diagonal Onsager processes except chemical osmosis

FEP 44 Chemical osmosis

FEP 50 Past burial history

FEP 55 Present-day stress regime

Hydro-mechanical coupling is important in many cases. It can be induced by:

- the drilling of the instrumentation borehole;
- the excavation of the tunnel;
- the subsidence/burial or uplift/erosion (or, more generally, stress) history of the site.

Only the latter is a natural hydraulic non-equilibrium situation. Depending on the hydraulic conductivity of the argillaceous formation and on the duration of the subsidence/burial or uplift/erosion process, this hydraulic non-equilibrium situation can persist many thousands (or even millions, see Nagra, 2002) of years. The amplitude of the consequent over- or underpressures also depends on the rate of the process.

Geochemical coupling is mentioned by several authors but little information was provided about the extent to which this effect could influence the measured hydrostatic potentials. Geochemical coupling could be an important factor for the length of the equilibration time in experiments, especially when the composition of the test fluid is very different from that of the pore-water.

A study in the Pierre Shale is worth mentioning (Neuzil, 2000). Fluid pressures and solute concentrations have been measured *in situ* for nine years and showed rapid head change (dm to m per year), which slowed to virtual constancy after 5 to 9 years. The pattern could be quantitatively interpreted as an initial pressure change due to chemical osmosis which slowed down as diffusion lowered the concentration gradient (see also FEPs 43 and 44).

Hydro-thermal coupling can also be important, as both the water and the matrix have a low compressibility (especially in indurated shales), although only very little information on this was provided. In the case of the head evaluation in Opalinus Clay in the Benken borehole, thermal effects were shown to be irrelevant (Nagra, 2002).

5.6 Level of understanding from a PA perspective and treatment in PA

From a PA perspective, the level of understanding is in general sufficient. Transport in the argillaceous formation is generally dominated by diffusion so that the head distribution in the formation is of relatively low importance. The head distribution in over- and underlying aquifers needs to be known (and can be more easily measured) in order to assess the dilution in those aquifers. Abnormal pressures are taken as evidence of a very low hydraulic conductivity over large scales in space and time, and thus serve to support the upscaling of measurements in boreholes.

Where sufficient knowledge is available, the hydraulic gradient over the argillaceous formation can be explicitly modelled in PA, and even the potential future evolution of the hydraulic gradient may be considered. However, because diffusion is the dominant transport process, the results of PA calculations indicate that the hydraulic gradient is not of high importance.

In formations where fracture flow occurs, the knowledge of the regional distribution of hydraulic potentials is more relevant.

5.7 Available reviews

None reported.

5.8 Planned work

IRSN plans to drill a new borehole penetrating the Toarcian-Domerian at Tournemire in 2004. One of the objectives is the characterisation of the head distribution.

5.9 Overall evaluation

This FEP is generally considered as relevant (we received a lot of detailed answers). Although the final influence on the repository performance could be very limited because of the negligible contribution of advection to transport through low permeability argillaceous formations, this FEP is very important for the understanding of the local and regional hydrogeological system (including the potential influence of water-conducting features).

6. HYDRAULIC PROPERTIES OF THE HOST ROCK (FEP A1.1.5)

6.1 Definition and generalities

Within the context of this FEP, the hydraulic properties of host rock include its ability to transmit water, variously evaluated as hydraulic conductivity, transmissivity or permeability, together with the spatial variation of these properties, and the dispersion length. For systems where fracture flow is important, effective porosity and fracture apertures must also be evaluated.

6.2 Site-specific experimental information

Formation/site	Type of information	Scale	Results and conclusions
Callovo-Oxfordian at Bure	Hydraulic parameters from packer tests and laboratory data on cores from deep drillings	Packer test intervals on a acale of 10 m. Laboratory data on cm to dm scale	Packer tests: K = 1.3 x 10^{-13} - 1.7 x 10^{-11} m/s, specific storage = 10^{-5} - 10^{-4} m^{-1}. Cores: K = 1 - 4 x 10^{-14} m/s. Transport is expected to be dominated by diffusion (Andra 1999a).
Toarcian-Domerian at Tournemire	*In situ* hydraulic tests and measurements on cores	cm to 10 m	Packer tests: K = 6.7 x 10^{-14} to 1.3 x 10^{-12} m/s, with highest values for fractured zones, specific storage = 10^{-7} to 10^{-6} m^{-1}. Cores: K = 10^{-14} m/s (Boisson *et al.* 1993, 1997, 1998, 2001).
Spanish Reference Clay in a Tertiary basin	Packer tests	cm to 10 m	K = 2.1 x 10^{-11} to 1.3 x 10^{-12} m/s Transport is expected to be dominated by diffusion (Lopez Geta *et al.* 1995).
Opalinus Clay in the Zürcher Weinland	Packer tests and measurements on cores	cm to 10 m	Packer tests: K = 1 x 10^{-14} to 6 x 10^{-14} m/s, specific storage 1 x 10^{-6} - 3 x 10^{-5} m^{-1}. Cores: K_h = 10^{-13}, K_v = 2 x 10^{-14} m/s. Transport is expected to be dominated by diffusion (Nagra, 2002). Modelling of the observed overpressures (FEP 5) suggests even smaller K values.

Formation/site	Type of information	Scale	Results and conclusions
Opalinus Clay at Mont Terri	*In situ* hydraulic tests and measurements on cores	cm to 10 m	K = 2 x 10^{-14} to 1 x 10^{-12} m/s storage = 1 to 5 x 10^{-6} m^{-1} (full range: 4 x 10^{-7} - 3 x 10^{-5} m^{-1}). Transport is expected to be dominated by diffusion (Bock, 2001).
Boom Clay at Mol	Packer tests, measurements on cores, large-scale simulation	cm to 10 m	K = 10^{-12} to 10^{-10} m/s, mean 2.2 x 10^{-12} m/s, anisotropy factor about 2, storage 0.9 to 1.8 x 10^{-5} m^{-1}. Transport is expected to be dominated by diffusion (Ondraf/Niras, 2002).
Boda Clay Formation at Mecsek	Packer tests	10 m	K = 1 x 10^{-10} to 1 x 10^{-12} m/s, minimum 10^{-13} m/s (fissured zones about a factor 100 larger, Ormai *et al*,. 1996, Csicsak, 1996).
Pierre Shale in south Dakota	Measurements on cores, borehole tests and large scale simulation	cm (cores), 10 m (borehole tests), basin scale for simulations	K= 1 x 10^{-14} to 1 x 10^{-10} (values above 10^{-13} m/s influenced by core damage, Neuzil, 1986).

In general very low hydraulic conductivities (i.e. below 10^{-10} m/s) are measured. The techniques to measure such low conductivities both on cores and in boreholes seem to be well established. Measurements in boreholes (packer tests) require high quality boreholes (borehole wall stability is often a problem) and very careful preparation, execution and analysis.

6.3 Scaling issues

Upscaling of hydraulic conductivity of argillaceous formations to the scale of a potential repository or to a regional scale is in general difficult. The scale of laboratory measurements is mostly limited to a few cm^3 or dm^3. Measurements in boreholes can be done in sections up to the full thickness of the studied argillaceous formation but the penetration depth into the formation during an injection test is generally very low (mm to dm). Measurements on the scale of tens of m^3 can only be done in underground research laboratories, e.g. by measuring the water inflow rate in large boreholes or gallery sections, often in combination with the measurement of the hydraulic gradient around the experimental section. Upscaling is then done by correlating (laboratory or borehole) measurements from different locations with lithology, granulometry and mineralogy.

Values of hydraulic conductivity derived from calibrations of regional scale hydrogeological models are in some cases larger than those from obtained from measurements (Ondraf/Niras, 2002). The reason for this difference remains currently mostly unexplained.

In Opalinus Clay in the Benken borehole, the observed hydraulic overpressures were modelled assuming hydro-mechanical coupling (Nagra, 2002). All calculations indicate that large-scale hydraulic conductivities lower than the measured ones are required to explain the preservation of the overpressures over long time scales. The preferred hypothesis to explain the scale-dependent values is a deviation from Darcy's law at hydraulic gradients <1, as they occur naturally in the formation. All hydraulic tests, both *in situ* and in the laboratory, were run with much higher gradients (typically thousands).

In the case of the Pierre Shale, regional permeabilities matched those measured in laboratory and borehole tests where the formation was at depths greater than about one km. Where the formation is closer to the surface, the regional permeability is 10^3 higher than values from core and borehole measurements. This is attributed to fracture zones separated horizontally by a km or more that are open near the surface but sealed at depth. (Neuzil & Belitz, 1998).

In formations where fracture flow is important, the upscaling of hydraulic conductivity is not trivial and depends on the size distribution, density, orientation and heterogeneity of the fractures. One possible route for upscaling is the calculation of large-scale effective hydraulic conductivities on the basis of fracture network models. For example, this approach was taken by Mazurek *et al.* (1999) for the highly consolidated and fractured marls at the Wellenberg site in the central Swiss Alps.

6.4 Scientific level of understanding

The hydraulic properties of the argillaceous formations studied are in general well understood at the scale of the measurements. No clear proof of deviations from Darcy's law have been found when measuring hydraulic conductivity, but most of the measurements were performed at much higher gradients than those prevailing in the field. The understanding of geochemical and geomechanical couplings and the role of fractures is in some cases still unsatisfactory. At larger, e.g. regional scale, the scientific level of understanding remains often rather low.

6.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 41	Swelling
FEP 42	Self-sealing
FEP 50	Past burial history
FEP 53	Past deformation events
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

6.6 Level of understanding from a PA perspective and treatment in PA

This FEP is mostly explicitly treated in the PA studies. From a PA perspective, the understanding of hydraulic properties is in general satisfactory. As the hydraulic conductivities are very low, transport, except in open fractures, is dominated by diffusion and so is insensitive to the value of hydraulic conductivity, hydraulic gradient as well as to coupled phenomena.

In fractured systems where advection is important, upscaling may be difficult and requires a good understanding of fracture geometries and of the connectivity of the fracture network.

6.7 Available reviews

Horseman *et al.* (1996).

6.8 Planned work

Further research work is planned mainly on upscaling the currently available data and determining the potential influence and/or presence of hydraulically conducting faults or fractures.

6.9 Overall evaluation

As argillaceous formations are in general studied because of their favourable hydraulic properties, i.e. a hydraulic conductivity that is so low that all transport is dominated by diffusion, this FEP is generally considered as highly relevant. It is mostly fairly well understood and the main uncertainties are related to geomechanical and geochemical coupling, upscaling and the (potential) role of faults and fractures.

7. UNITS OVER- AND UNDERLYING THE HOST FORMATION: LOCAL AND REGIONAL HYDROGEOLOGIC FRAMEWORK (FEP A1.1.6)

7.1 Definition and generalities

The features described in this FEP establish the hydraulic, chemical and thermal boundary conditions for the host rock. They are also likely to be the units through which rapid transport to the biosphere would occur for any radionuclide escaping from the host rock.

7.2 Site-specific experimental information

Formation/ site	Type of information	Scale	Results and conclusions
Callovo-Oxfordian at Bure	Hydrogeological characterisation of over- (Oxfordian) and underlying (Dogger) limestone formations belonging to the Paris Basin, which has been intensively studied (e.g. surface studies, large number of boreholes)	Local and regional (basin scale)	The limestones over- and underlying the Callovo-Oxfordian are regional aquifers (Andra, 1999a). Flow directions are towards the centre of the basin, i.e. to the W in the region of interest.
Toarcian-Domerian at Tournemire	Hydrogeological characterisation of over- and underlying limestone formations; local head and permeability measurements	Local scale	Upper limestone formation is a local aquifer, lower limestone formation is an important regional aquifer (Boisson *et al.*, 1998).
Spanish Reference Clay in a Tertiary basin	Boreholes, surface outcrops	Local scale	The host formation is overlain by *ca.* 100 m low-permeability marls with gypsum. Aquifers are located above this unit as well as below the base of the host formation (Lopez Geta *et al.*, 1995).

Formation/ site	**Type of information**	**Scale**	**Results and conclusions**
Opalinus Clay at Mont Terri	Pore-water compositions derived from a series of short boreholes drilled from the safety tunnel (profile across the Opalinus Clay and the embedding units)	Local	The Opalinus Clay is overlain by Dogger limestones and underlain by Liassic marls and limestones and by Keuper marl and Gipskeuper. Pore-water salinity, ^{18}O, ^{2}H and He contents are greatest at Opalinus Clay-Liassic contact and decrease smoothly to low values in Dogger and Keuper limestone aquifers. The distribution of solutes and isotopes on Opalinus Clay and underlying marls is consistent with diffusion to the overlying and underlying fresh-water aquifers (Pearson *et al.,* 2003).
Opalinus Clay in the Zürcher Weinland	Boreholes with permeability and head measurements, ground-water residence times, hydro-geochemistry, surface outcrops	Local and regional	The host formations (Opalinus Clay + Murchisonae Beds) are embedded within confining units, which are dominated by argillaceous, low-permeability formations but contain potentially water-conducting beds or local aquifers. The confining units over- and underlying the host formations are 100 and 150 m thick and are bounded by the regional aquifers (Malm and Muschelkalk). The regional aquifers show hydrostatic conditions, whereas slight over- and underpressures are observed within the confining units (Nagra, 2002).
Boom Clay at Mol	Head measurements, permeability, geochemistry (including isotopes), residence time, hydrogeological model at different scales	Local (350 km^2) up to regional (6 000 km^2)	The overlying Neogene aquifer is a very important regional aquifer that is heavily exploited. The underlying units include sand layers separated by a clay layer (Asse aquitard). These aquifers are more saline, and residence times show a palaeoclimatic signal (influence of glaciations) Ondraf/Niras, (2002).
Boda Clay Formation at Mecsek	Overlying Permian sandstone: head measurements, permeability, hydro-geochemistry, hydrogeological model	Local scale	Sandstones form an aquifer (Ormai *et al.,* 1996).
Pierre Shale in south Dakota	Underlain by regional Dakota Sandstone aquifer	Regional	Distribution of regional vertical transmissivity of shale deduced from flow modelling of aquifer (Neuzil & Belitz, 1998).

Formation/ site	Type of information	Scale	Results and conclusions
Mizunami Group at Tono	The overlying formation is the Seto Group, an unconsolidated fluvial facies, the underlying formation is the Toki biotite granite; permeability and geochemical data		The Seto Group is permeable (hydraulic conductivity 10^{-6} to 10^{-7} m/s), The Toki granite has a hydraulic conductivity of 10^{-9} to 10^{-7} m/s. Reference: Hama *et al.* (1995).

In most cases the argillaceous formations studied are found in large sedimentary basins and thus fall in a sequence of other geological layers of sedimentary origin (limestones, sandstones, sands, marls...). Each such sequence generally corresponds to a sequence of regional aquifers and aquitards. The aquifers can be rather easily characterised by using classical hydrogeological techniques, provided a sufficient number of observation points is available. Regional hydraulic properties of the target formation may be inferred from the hydrogeology of bounding aquifers. The geological history and evolution of the target formation may be evident in the patterns of geochemical change through the formation to bounding aquifers.

In most cases, the host formations are located directly between aquifers. In contrast, the Opalinus Clay in the Zürcher Weinland is embedded within low-permeability confining units, which separate it from the regional aquifers.

7.3 Scaling issues

Within a sedimentary basin, the geological layers often have a large lateral extent, which makes upscaling from local to regional scale relatively easy. For this purpose, in most cases a combination is made of (core) drillings, geophysical logging techniques and seismic investigations spread over the region of interest.

At least in the case of the Opalinus Clay in the Zürcher Weinland, the situation is more complex, and local and regional aquifers have spatially variable properties:

- The overlying Malm is a regional aquifer but has very low hydraulic conductivity in the Benken borehole. A very old (at least hundreds of ka) Na-Cl water was sampled. This limestone aquifer is known to be spatially variable due to heterogeneous fracturing and/or degree of karstification.
- The underlying, local aquifer in the Keuper has a high hydraulic conductivity in the Benken borehole, even though the residence time of the water is >25 ka. Lateral variations of the sedimentary facies (and also of hydraulic properties) are known, and the findings from the Benken borehole cannot be extrapolated to large horizontal distances (more than a few km).

Depending on regional evidence, the local hydraulic conductivities measured in the Benken borehole were upscaled and resulted in both higher and lower regional values (Nagra, 2002).

7.4 Scientific level of understanding

In general the properties and the behaviour of the over- and underlying units and their role within the regional and local hydrogeological framework are well understood. The main remaining uncertainties are related to the assessment of water fluxes through the aquitards.

7.5 Linked FEPs

FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 50	Past burial history
FEP 53	Past deformation events

7.6 Level of understanding from a PA perspective and treatment in PA

From a PA perspective, aquifers are considered:

1) to define the hydrogeological and hydrochemical boundary conditions for flow and transport within the host formations, and
2) as potential exfiltration pathways for radionuclides, where dilution is taken into account.

In general the level of understanding of the local and regional hydrogeological framework is sufficient to assess the dilution and radionuclide fluxes that might end up in the aquifer system, as well as to evaluate the boundary conditions for processes within the host unit.

The local and regional hydrogeological system is explicitly treated in many PA studies. In many cases regional 3-D or quasi-3-D hydrogeological models have been applied to simulate the regional ground-water flow and to determine the boundary conditions for local-scale models. Regional-scale models have also been applied to assess the influence of potential climate changes on the hydrogeological framework. The local-scale models were mainly used to determine the dilution and fate of radionuclide fluxes that might enter the aquifer system.

In the case of the Opalinus Clay, retention within the confining units which embed the host formations is neglected in the base case of PA, i.e. direct exfiltration into the aquifers is assumed. Alternative cases calculate the retardation in these units in a simplified way.

7.7 Available reviews

None reported.

7.8 Planned work

None reported.

7.9 Overall evaluation

This FEP is generally well understood both from a scientific and PA perspective. In many cases comprehensive studies have been made on it and the research techniques for it are well established.

8. DIFFUSIVITY (FEPS A1.2.1, A2.1.1)

8.1 Definition and generalities

Diffusion occurs in all argillaceous media, both natural clay and shale being considered as a potential host rock, and in plugging and backfill material, particularly compressed bentonite. Diffusion is relevant to the far field in connection with site characterisation and nuclide transport properties for PA and to the affected field as boundary conditions for analysis of the engineered barrier system.

Different definitions of the terms “diffusivity” and “diffusion coefficient” applied to molecular transport in porous media (rocks) exist in the literature. Special care must be taken with these definitions when comparing reported rock properties and performing quantitative computations of diffusive transport.

For describing diffusion in water-saturated porous media, two types of diffusion coefficients must be distinguished: the effective diffusion coefficient (D_e) appropriate for Fick’s first law, and the apparent diffusion coefficient (D_a), used with Fick’s second law. Following the definitions of Horseman *et al.* (1996), which are widely used:

$$D_e = n_d\,(\chi/\tau^2)\,D_0 = n_d\,D_p \qquad (1)$$

where n_d is the species-specific diffusion porosity (see FEP 9), D_0 the free-water diffusion coefficient appropriate for the species and fluid chemistry of interest, and (χ/τ^2) the rock-specific geometry factor. D_p is the rock- and species-specific pore diffusion coefficient.

$$D_a = D_e / (n_d\,R) = D_p / R \qquad (2)$$

where R is the retardation factor:

$$R = 1 + (\rho_d\,K_d / n_d). \qquad (3)$$

ρ_d is the dry density of the sample and K_d the distribution coefficient of the species (see FEPs 14-22, A2.2 series). For non-retarded species, $D_a = D_p$ so D_p may be used in modelling the distribution of non-retarded substances.

The term “diffusivity” is variously used to mean, for example:

- Diffusion coefficient, e.g. effective and apparent diffusivities.
- Apparent diffusion coefficient.
- The diffusional tortuosity.

Thus, if the term is used, it should be precisely defined.

8.2 Site-specific experimental information

A number of measurements of the diffusion coefficients of argillaceous formations have been reported. The following table (based on Nagra, 2002) summarises the results of laboratory tests on formations of nuclear-waste interest. These all represent properties of the bulk matrix. No direct measurements of diffusion properties that cause retardation of solute transport in fractures were reported. Constraints on diffusion coefficients can also be obtained from the quantitative evaluation of natural tracer profiles across the host formations, and these aspects are described in FEP 24.

Formation/ site	**Tracer**	**No. of tests**	**D_e parallel (‖) or perpendicular (⊥) to bedding [x 10^{-11} m^2/s]**	**Porosity [-]**	**Reference**
Callovo-Oxfordian at Bure	^{3}H ^{125}I^{-}	24 5	⊥ 1.4 ⊥ 0.12	0.1 - 0.2	Andra (1999a)
Toarcian-Domerian at Tournemire	^{3}H I^{-}	16 4	⊥ 0.4 ⊥ 0.02	0.02 - 0.2 -	Boisson *et al.* (1998), Savoye *et al.* (2001), Cabrera *et al.* (2001)
Spanish Reference Clay in a Tertiary basin	^{3}H Cl^{-}		⊥ 10 - 12 ⊥ 2.9 - 6.8		Tests made on samples reconstituted to higher density than in field
Opalinus Clay at Mont Terri	^{3}H I^{-}	14 9	⊥ 1 - 2 ⊥ 0.3 - 0.4	0.10 - 0.25 0.06 - 0.15	Nagra (2002)
Opalinus Clay in the Zürcher Weinland	^{3}H ^{36}Cl^{-}	3 3	⊥ 0.5 - 0.7 ⊥ 0.07 - 0.09	0.13 - 0.15 0.03 - 0.04	Nagra (2002)
Boom Clay at Mol	^{3}H	4	⊥ 8 - 11 ‖ *ca.* twice ⊥	0.46±0.02 at 0.02 M Cl^{-} 0.59±0.07 at 1.0 M Cl^{-}	De Cannière *et al.* (1996)
	I^{-}, Br^{-}	10	⊥ 2 - 6	Br^{-}: 0.18±0.03 at 0.02 M Cl^{-} I^{-}: 0.19±0.01 at 0.02 M Cl^{-} I^{-}: 0.30±0.09 at 1.0 M Cl^{-}	
Palfris Formation at Wellenberg	^{3}H I^{-}	1 1	⊥ 0.2 ⊥ 0.01	0.03 0.009	Lineham & Stone (1991), Pearson (1999)
London Clay (UK)	^{3}H, ^{2}H I^{-}	14 3	⊥ 7 - 9 ⊥ 3 - 5	0.56 - 0.62 0.21 - 0.31	Bourke *et al.* (1993)
Water	^{3}H		226	Self-diffusion coefficient	Atkins (1990)

Extensive sets of measurements of the diffusion properties of the Opalinus Clay at Mont Terri are summarised by Tevissen & Soler (2003) and in Table 5.10-1 of Nagra (2002). Measurements were made both perpendicular and parallel to the bedding with several tracers under various confining conditions at a number of laboratories. From these it can be concluded that:

- The effective diffusion coefficient for HTO is in the range of 1 – 2 x 10^{-11} m^2/s perpendicular to the bedding and 5 – 10 x 10^{-11} m^2/s parallel to it.
- The diffusion-accessible porosity for HTO is the same as the total porosity of the rock, considering the uncertainties in its measurement by laboratory diffusion tests.
- Effective diffusion coefficients and accessible porosities for Cl^-, Br^- and I^- are smaller by factors of 10 and 3, respectively, than corresponding values for HTO. These differences are consistent with the anion exclusion process (FEP 10).
- Confining pressures exerted perpendicular to the bedding seem to have no effect on the properties of diffusion parallel to the bedding.
- The results are for samples taken from throughout the formation at Mont Terri. Their consistency indicates that there is little spatial variability in the diffusion properties of the formation.

Diffusion data measured on core samples of the Opalinus Clay from the Benken borehole are described by Van Loon *et al.* (2003) and summarised in Table 5.10-2 of Nagra (2002) as follows:

Tracer	**⊥ or ‖**	**Number of tests**	**D_e [x 10^{-11} m^2/s]**	**Porosity [-]**	**Comments**
^{3}H	⊥	8	0.61±0.1	0.13 - 0.15	4, 8, 14, 15 MPa confining pressure
	‖	2	3.15±0.05	0.13 - 0.15	14 MPa confining pressure
$^{36}Cl^-$	⊥	3	0.08±0.01	0.03 - 0.04	4, 8, 15 MPa confining pressure
$^{125}I^-$	⊥	3	0.05±0.02	0.06 - 0.08	4, 8, 15 MPa confining pressure; relatively higher porosity then ^{36}Cl explained as weak sorption

Diffusion properties of several argillaceous formations have been measured in borehole tests and by modelling in situ diffusion profiles. These are shown in the following table.

Formation/ site	**Method**	**Sub-stance**	**Diffusion coefficient [m^2/s]**	**Porosity [-]**	**Comment/ reference**
Opalinus Clay at Mont Terri	Numerical analysis of ^{4}He injection	^{4}He	D_e: 2.1 x 10^{-11}	0.30	FM-C Experiment, Tevissen & Soler (2003)
Opalinus Clay at Mont Terri	Numerical analysis of concentration changes of tracers in borehole fluids and distribution in surrounding formation sampled by overcoring	HTO	D_e: 5 x 10^{-11}	0.15	DI Experiment, Tevissen & Soler (2003)
		I^-	Unequivocal interpretation not possible because of I^- retention either in borehole or formation		
Opalinus Clay at Mont Terri	Analytical evaluation of *in situ* profiles led to D_a values shown. D_e values calculated using assumed porosities	^{2}H, ^{18}O	D_a: 7 x 10^{-11} D_e: 1.4 x 10^{-11}	0.2 assumed	Degueldre *et al.* (2003)
		Na^+	D_a: 2.5 x 10^{-11} D_e: 0.5 x 10^{-11}	0.2 assumed	
		Cl^-, Br^-	D_a: 2.5 x 10^{-11} D_e: 0.25 x 10^{-11}	0.1 assumed	
		^{4}He	D_a: 3.5 x 10^{-11} D_e: 0.7 x 10^{-11}	0.2 assumed	Rübel *et al.* (2002)
Pierre Shale in south Dakota	Numerical analysis of concentration changes in borehole fluids		Ionic diffusivity $D_a = 10^{-11}$ to 10^{-12}	0.29 to 0.35	Neuzil (2000)

In the Toarcian-Domerian at Tournemire, fracture flow occurs at least on a small scale. Tracer profiles from fractures into the rock matrix were identified with a penetration depth of *ca.* 1 m, even though the shape of the profiles is complex and cannot be explained in terms of one single event or process (Patriarche, 2001).

In some of Andra's experiments in the framework of the investigations of the Callovo-Oxfordian at Bure, the diffusion coefficient for cations was higher than expected. Either K_d values chosen for the evaluation were too high, or other processes such as surface diffusion play a role.

Electrical conductivity logs in boreholes have been used by the oil industry to constrain formation factors mostly in sand-rich formations (the main goal being the determination of the degree of water saturation, see e.g. Worthington, 1985). Other studies derive diffusion properties from measurements of electrical conductivity (e.g. Revil *et al*,. 1997). All these methods are not specific to clay-rich systems, and it is not clear if the different processes acting in argillaceous rocks can be satisfactorily separated to allow clear conclusions.

8.3 Scaling issues

Most data are based on laboratory tests at cm scales. Field experiments may be possible at m scales, but often not at dam or hm scales required for PA (Put & De Preter, 1997). Only concentration profiles of natural tracers are available at those scales. To upscale laboratory data requires information about the distribution and homogeneity of diffusion-affecting formation properties, and should be tested as far as possible using *in situ* tests and natural tracers.

In the Opalinus Clay at Mont Terri and in the Benken borehole, the laboratory-derived diffusion coefficients are consistent with those calculated for the natural tracer profiles (FEP 24). In the Toarcian-Domerian at Tournemire, this is not the case. At other sites, such a comparison has not yet been addressed specifically. While uncertainties exist in the choice of boundary and initial conditions for the quantitative interpretation of large-scale tracer profiles, the constraints are sufficient for a meaningful result in some cases.

8.4 Scientific level of understanding

The theory of diffusion in homogeneous media is well understood, but the modelling of diffusive fluxes in heterogeneous materials with charged surfaces, large surface areas and very small pores is still not fully resolved. Furthermore, except for solutes of simple chemistry in formations demonstrably homogeneous such as the Boom Clay or Opalinus Clay, there are open questions about practical, reliable techniques to choose parameter values for modelling diffusion on the repository scale. Knowledge provided by laboratory experiments and field tests is sufficient only for a constrained extrapolation in space and time. Natural tracer profiles can be used to reduce existing uncertainties.

8.5 Linked FEPs

FEP 9	Connected matrix porosity
FEP 10	Ion exclusion
FEP 11	Surface diffusion

Evaluating the parameters for calculating diffusive flux requires consideration of:

FEPs 14-22 Sorption (A2.2 series).

8.6 Level of understanding from a PA perspective and treatment in PA

Because diffusion is an important transport mechanism in all types of argillaceous rocks, it is usually modelled explicitly for PA. In unfractured rock, diffusion is likely to be the dominant transport mechanism. In some fractured formations, advection in the fractures may dominate, but diffusion into the matrix will be an important retardation mechanism.

Various combinations of parameter values may be required for PA modelling. D_a and/or D_e values based on laboratory and field experiments may be specified directly for each solute of interest. Alternatively, D_p values along with R or K_d values for each solute may be given. The former are derived from experiments using non-retarded solutes, and the latter are based on considerations given in FEPs of the A2.2 series (sorption, broad definition). Care must be taken when extrapolating retardation coefficients calculated using batch K_d values to *in situ* conditions.

Refinements in modelling, such as variations in diffusion properties with depth, location or direction, can be included if site data warrant.

8.7 Available reviews

Considerations in diffusion modelling and parameter determination and selection are reviewed by Horseman *et al.* (1996) and in textbooks on geochemical processes such as those of Lerman (1979) and Lasaga (1998). The classic work on diffusion calculations is that of Crank (1975).

Site specific reviews include those for the Opalinus Clay at Mont Terri by Tevissen & Soler (2003) and for the Opalinus Clay in the Benken borehole, the Mont Terri underground research laboratory and for other argillaceous formations in Nagra (2002, Sect. 5.10).

8.8 Planned work

In situ tracer tests and observations of natural tracer concentration patterns are underway or planned at Mol and Bure.

8.9 Overall evaluation

As the diffusion coefficient is a very sensitive parameter in PA, this FEP is highly relevant. The process is very well understood for non-retarded solutes with simple chemistry, but less so for retarded solutes. Site specific laboratory and field experimental studies will generally be needed to assure that correct values are available for PA. There is particular uncertainty in parameter values required for modelling retardation of fracture transport by matrix diffusion.

9. CONNECTED MATRIX POROSITY (FEPS A1.2.2, A2.1.2)

9.1 Definition and generalities

This FEP applies to all repository concepts that include media rich in clay minerals in the near or far fields, but explicitly excludes fracture porosity, which is considered in FEP 3. It is relevant to the far field in connection with site characterisation and nuclide transport properties for PA and to the affected field as boundary conditions for analysis of the engineered barrier system.

Connected matrix porosity is that proportion of the total rock volume that forms continuous pathways through a rock mass allowing possible (albeit possibly perhaps highly tortuous) flow paths through the domain being considered. The distinction between total and interconnected, and between matrix and fracture types of porosity is important for transport calculations in argillaceous formations. The total connected matrix void space will contain some immobile pore-water, i.e. water bound to mineral surfaces and clay-mineral interlayers and non-advecting water in dead-end pore space. Such water will not take part in dispersive and advective transport processes, but may be involved in diffusive processes. Hence connected matrix porosity should be differentiated from effective or kinematic porosity, which is the connected porosity involved in advection and dispersion. The current terminology used to describe various types of porosity is confused and non-standardised. For example, connected porosity (which includes dead-end pore space) is also termed effective porosity by some authors (e.g. Domenico & Schwartz, 1990), while other authors consider effective and kinematic porosity to exclude dead-end pore space (e.g. Horseman *et al.*, 1996) and hence to represent a proportion of connected porosity. The latter definition is also consistent with the definition of the effective diffusion coefficient adopted in FEP 8. The types of porosities found in argillaceous formations are discussed by Pearson (1999) using the same definitions as Horseman *et al.* (1996). These definitions are also adopted in this report.

9.2 Site-specific experimental information

Formation/site	Porosity value and type	Comment	Reference
Callovo-Oxfordian at Bure	Water-content porosity at 105 °C: 0.15 ^{3}H-accessible porosity: 0.15; similar values for cations (Cs, Na) Mercury injection: 0.12		
Toarcian-Domerian at Tournemire	Densitometry: 0.04 - 0.09 Accessible to HTO: 0.06 - 0.11, with some outliers Mercury injection and BET isotherms: 0.08 - 0.11		Boisson *et al.* (1998)
Spanish Reference Clay in a Tertiary basin	Water-content porosity at 105-110 °C: 0.34 - 0.45	Porosity decreases with depth due to increasing compaction	
Opalinus Clay at Mont Terri	Water-content porosity at 105-110 °C: 0.13 - 0.19 Through diffusion: HTO: 0.9 - 0.22 Halide: 0.05 - 0.14	Cl porosity from pore-water samples and leaching: 0.05 - 0.15	Pearson *et al.* (2003), Annex 10
Opalinus Clay in the Zürcher Weinland	Water content porosity: 0.108±0.019 Through diffusion: HTO: 0.14 Cl^- : 0.04	Diffusion porosity by water isotope mass balance: 0.130±0.015	Nagra (2002)
Boom Clay at Mol	Diffusion accessible porosity: 0.1 to 0.3, depending on the species and consolidation pressure. *in situ* value ≈ 0.35 for HTO and ≈ 0.1 for I^-	Determined for radionuclides on small (cm scale) clay cores in the laboratory and confirmed in large-scale (1 to 10 metres) *in situ* experiments	Ondraf/Niras (2002), Tab. 11.3.8-4
Pierre Shale in south Dakota	Total porosity: 0.29 to 0.35	Determined from borehole gravimetry and shale densities as function of depth	Neuzil (1993)
Palfris Formation at Wellenberg	Water content porosity 0.029±0.010 Hg porosimetry 0.033±0.012	Cl^- porosity from borehole sample and leaching; 0.009	Baeyens & Bradbury (1994); Nagra (1997)

Formation/site	Porosity value and type	Comment	Reference
London Clay, (UK)	Water content porosity *ca.* 0.6; HDO, HTO through- and out-diffusion porosity 0.60±0.05	I^- through- and out-diffusion porosity 0.27±0.06	Bourke *et al.* (1993)
Various argillaceous formations in UK	St Bees Shale:		Nirex reports
	0.01 - 0.08	Liquid resaturation	
	London Clay:		
	0.33 - 0.48	Oven drying (water content)	
	0.19 - 0.49	Solute out-diffusion	
	0.33 - 0.57	Small angle neutron scattering	
	Oxford Clay:		
	0.5±0.05	Diffusion experiments	

Porosities are found routinely from density and specific gravity measurements, from water-loss measurements, using fluid (e.g. He or Hg) injection techniques and during the measurement of diffusion parameters. Discussions of these (and other) methods are given by Pearson *et al.* (2003, Annex 10), Nagra (2002) and Bourke *et al.* (1993).

Due to the complex structure of the pore space and due to the interactions between water, solutes and clay-mineral surfaces, different methods may yield somewhat different porosity values even for identical samples. These systematic differences are well understood at least for some of the formations considered here (see, for example, Pearson *et al.*, 2003 for Opalinus Clay at Mont Terri). In addition to the methodological issues, matrix porosity also varies as a function of the solute considered. While porosity accessible to water is thought to represent the total interconnected matrix porosity, anions can only move in a fraction of the water-accessible pore space due to electrostatic interactions with clay surfaces (see FEP 10, ion exclusion). Thus porosity values for argillaceous rocks should always be related 1) to the measurement technique and 2) the solute in question.

The table includes values for the Cl porosity of some of the formations considered. This property, which is also referred to as the *geochemical porosity* (Pearson, 1999), is found by comparing the Cl content of the bulk rock, determined by aqueous leaching, with that of squeezed water or borehole samples of pore-water.

9.3 Scaling issues

Laboratory and borehole measurements represent scales of cm and m, respectively. For unfractured, homogeneous media (e.g. Boom Clay) such measurements may be directly applicable for PA. For inhomogeneous media, such as formations consisting of different lithologies or containing abundant fracture-infill materials, the 3-D architecture of the host rock must be known in order to be able to upscale laboratory data.

Interdependence of porosity and diffusion properties may permit inference of porosity distribution from interpretation of distribution of natural tracers.

9.4 Scientific level of understanding

The concept of porosity is well understood, although practical problems can arise when considering the meaning of different porosity values (e.g. bulk, interconnected, effective, geochemical, etc.) in terms of radionuclide transport, and when interpreting the results of various measurement techniques. Different porosities are required for different objectives (e.g. advective water flow or diffusion of a specific solute) and care must be taken to select the one based on the appropriate experimental technique (see FEP series A1.2 & A2.1).

The correspondence of various methods used to evaluate porosity (e.g. wet *vs.* dry densities, Hg and gas porosimetry, diffusion techniques, borehole gravimetry, neutron logging, formation factors) and of the several types of pore-water in argillaceous formations (e.g. interlayer water surface-bound water, unstructured "free" water) with the advective and diffusive transport and geochemical properties are much less well understood for argillaceous formations than for coarsely crystalline or coarse-grained sedimentary rock types.

9.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture water composition
FEP 18	Dissolution/precipitation of solid phases
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 33	Thermally induced consolidation of the host rock
FEP 50	Past burial history
FEP 58	Consolidation due to burial

9.6 Level of understanding from a PA perspective and treatment in PA

At a large scale, connected matrix porosity is one of the key parameters governing the diffusive and advective transport properties of the host layer. The uncertainty regarding the transfer time through the formation is linked to the uncertainty possibly affecting the evaluation of this parameter.

The formative processes (primary and diagenetic) are well understood, leading to a reasonable expectation of the degree of spatial variability. The impact of connected porosity on radionuclides relates to both transport and retardation mechanisms. Conceptually, the impact that connected matrix porosity has in relation to both components is understood, although detailed properties such as the sorption for individual species, may not be. Quantitative evaluation of connected matrix porosity for transport and retardation experiments is well described for individual samples at the laboratory scale, but is considered scale dependent. Upscaling requires knowledge of the spatial arrangement of lithologies and fracture-infill materials within heterogeneous formations.

In fractured media, the accessibility of the fluid to the adjacent parts of a potential water-conducting structure depends on the connected matrix porosity. Variability of connected matrix porosity, and therefore the diffusion length inside the porous blocks, have an important influence on effective transit time of the fluid throughout migration pathways.

Diffusion accessible porosity is a key parameter for the calculation of transport in Boom Clay. The parameter is sensitive but well understood. For the Boom Clay there is experimental evidence that the Bruggeman equation (or the more general Ayres equation) is valid (De Cannière *et al.*, 1996). This power law equation relates the effective diffusion constant to the diffusion accessible porosity.

9.7 Available reviews

The types of porosity found in argillaceous formations are described by Pearson (1999). The types of porosity in the Opalinus Clay and relevant to safety assessment are discussed by Nagra (2002).

9.8 Planned work

None reported.

9.9 Overall evaluation

Diffusion is likely to be a major transport mechanism for release from a repository in an argillaceous host rock. Thus, all parameters relevant to its modelling must be known, including, among others, connected matrix porosity. The uncertainty in determining or estimating connected matrix porosity values is likely to be small relative to the uncertainties in values for diffusion coefficients and concentration gradients that will be used for PA.

Evaluations of connected and effective porosity are important for PA and for site characterisation. The status of conceptual knowledge is adequate, but site specific studies at a variety of scales are essential. In addition, techniques used to upscale/downscale and investigate retardation mechanisms in relation to interconnected porosity are necessary.

In some PA analyses, neither pore size distributions nor solute-specific accessible porosities are direct input parameters for PA calculations. Thus, strictly for such PA purposes, it may not be necessary to determine solute-specific accessible porosity. Instead, the effective and apparent diffusion coefficients (D_e and D_a) could be measured because they are the parameters that really appear in the transport equations.

10. ION EXCLUSION (FEPS A1.2.3, A2.1.4)

10.1 Definition and generalities

The membrane properties of argillaceous rocks are such that ions are excluded to a greater extent than similarly-sized uncharged solutes. As argillaceous formations are compacted, the double layers of adjacent platelets approach and the pore space between them develops a negative charge, which prevents anions from migrating through them. Cations are also restrained by the requirement that the pore fluid remain electrically neutral. Uncharged solvent and solute molecules are able to pass through charged pores, but ions are excluded. This process is known as Donnan exclusion (Fritz, 1986; Horseman *et al.*, 1996).

As discussed in FEP 17, the geochemical, or free-water, porosity is required to find the salinity of pore-water from bulk leaching data when the water cannot be sampled directly. The porosity from which ions are not excluded corresponds to its geochemical or free-water porosity (Pearson 1999). The extent to which ions are excluded increases with compaction. It decreases with the salinity of the pore-water because the thickness of the double layer decreases as salinity increases.

Ion exclusion affects a number of diagonal and off-diagonal Onsager transport processes, such as diffusion, chemical osmosis or hyperfiltration (FEPs 8, 43, 44).

10.2 Site-specific experimental information

Several types of studies of the membrane properties of argillaceous rocks have been carried out that are relevant to nuclear waste site characterisation and PA.

Laboratory studies of diffusion in a number of argillaceous rocks are described in FEP 8. Comparison of the effective diffusion coefficients from these studies shows the extent to which ions will be excluded relative to other ions during diffusion.

Laboratory and field studies of osmosis in samples of Opalinus Clay from Mont Terri, and borehole studies in the Pierre Shale are described in FEP 44. These provide data on osmotic efficiencies that can be used to evaluate ion exclusion associated with advection.

Finally, one study of hyperfiltration of uncharged solutes is also under way. Natural organics that can affect nuclide transport are found in the pore-water of the Boom Clay (FEP 17). The chemistry of the Boom Clay pore-water shows that the formation has been flushed by fresh water, yet the organics remain. Studies of Boom Clay core are now in progress testing the hypothesis that this retention of organics is a result of hyperfiltration or possibly ion exclusion.

10.3 Scaling issues

The theory of diffuse double layers applies at the microscopic scale. Effective diffusion coefficients and diffusion porosities are based on laboratory studies carried out at the scale of centimetres. The scale relevant for PA is several tens of metres. In homogenous rock, no significant scale effects are to be expected. Nevertheless, the validity of upscaling has to be verified by *in situ* tests, such as studies of natural tracer concentration profiles of chloride and bromide and by precise characterisation of lithologic variability.

10.4 Scientific level of understanding

Although ion exclusion is well-known in principle, the effect of salinity variations on diffusion, and a description of anionic exclusion at a microscopic level is needed.

The formation of diffuse double layers with a deficiency of negative charge (deficiency in anion concentration) and an excess of positive charge (excess cation concentration) has a good theoretical basis (e.g. Sposito, 1984). The former provides good qualitative understanding of the macroscopic effect of anionic exclusion on diffusion. Cation exclusion is explained as the result of electrostatic coupling between cations and anions in order that positive and negative charges will be balanced during transport. However, it is not clear that this restriction applies to transport of a tracer, which could occur by an exchange mechanism (e.g., diffusion of K^+ in an argillaceous formation containing an NaCl pore-water).

10.5 Linked FEPs

FEP 9	Connected matrix porosity
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture-water composition
FEP 29	Interactions of hyperalkaline fluids and host rock

10.6 Level of understanding from a PA perspective and treatment in PA

In unfractured argillaceous formations, diffusion is the dominant transport mechanism. In models used directly for PA, effective and/or apparent diffusion coefficients are used directly. Values for these coefficients are commonly laboratory values, but field experiments and natural tracer studies may also provide quantitative information. Ion exclusion information and ion-specific diffusion porosities are used to calculate pore diffusion coefficients which are used in some PA calculations. In addition, they are used to support estimates of diffusion coefficients for unmeasured species and, as geochemical porosities, to support the calculation of pore-water salinity and chemistry in formations too tight for direct sampling.

10.7 Available reviews

Horseman *et al.* (1996), Soler (1999, 2001).

10.8 Planned work

None reported.

10.9 Overall evaluation

Ion exclusion results in differences in the porosity accessible for transport of solutes of various charges and sizes. It is important in describing diffusive transport, in the membrane and osmotic properties of argillaceous rocks and in quantifying the pore-water chemistry. Diffusion-accessible porosities may be used directly in PA transport calculations as necessary support for choosing PA diffusion parameter values.

11. SURFACE DIFFUSION (FEPS A1.2.4, A2.1.5)

11.1 Definition and generalities

Diffusion rates and apparent diffusion coefficients (D_a) measured for sorbing cations such as Cs^+ and Sr^{+2} in compacted bentonite may be higher than values calculated using batch distribution coefficient (K_d) values (see FEP 8, eq. 2 & 3). The difference has been explained either by arguing that distribution coefficients in the compacted bentonite are smaller than those measured in batch experiments, or by proposing the existence of an additional transport mechanism. The latter process, surface diffusion, postulates that a fraction of the cations close to the clay-mineral surfaces are still mobile (able to move along the surfaces), and contribute to the total diffusive flux of cations.

Surface diffusion may be relevant to the far field in connection with site characterisation and nuclide transport properties for PA and to the affected field as boundary conditions for analysis of the engineered barrier system.

It could also be the case that values for the pore diffusion coefficient (D_p) or porosity (n) used to calculate the expected diffusion properties are incorrect. The values used are usually those measured using non-retarded anions or water isotope tracers (HDO, HTO), and could well be inappropriate for calculating cation properties. Certainly, anion porosities are smaller than those for water itself (FEP 9).

If surface diffusion does occur, the measured effective (D_{em}) and apparent (D_{am}) diffusion coefficients can be considered to include pore diffusion (D_p) and surface diffusion (D_s) contributions acting in parallel so they can be summed (Horseman *et al.* 1996, Lehikoinen 1999):

$$D_{em} = n\,D_p + (1 - n)\,\rho_d\,K_d\,D_s \tag{1}$$

can be combined with the retardation factor $R = 1 + \dfrac{\rho_d K_d}{n}$ to obtain

$$D_{am} = \frac{D_{em}}{n\,R} = \frac{n\,D_p + (1-n)\,\rho_d\,K_d\,D_s}{n + \rho_d\,K_d}\,. \tag{2}$$

This formulation assumes that surface diffusion is uniform across the part of the cross-section of the clay which is occupied by minerals. The surface diffusion coefficient (D_s) is thus an averaged parameter of no fundamental significance.

The proposed mechanism of surface diffusion has not been well described. It seems unlikely that the phenomenon observed involves movement of ions or molecules that are chemically bound to mineral surfaces by surface complexation or ion exchange. A more plausible explanation would be that cations which can take part in an ion exchange process are not “sorbed” at specific sites at the mineral surface. Instead, they may be those that occupy the diffuse layer in the vicinity of the surface and, thus, are still mobile. The ion mobility in this layer may be lower than in ordinary water because of the higher viscosity of the water layer adjacent to the clay-mineral surface.

Horseman *et al.* (1996) conclude that discrepancies between measured and calculated diffusion properties can be explained as the result of using inapplicable parameter values for calculating the expected properties. Thus, they see no need to invoke surface diffusion as a process of real concern. In support of this conclusion, they cite Oscarson (1994) who concluded that batch-measured distribution coefficients may be too high and lead to calculated diffusion coefficients lower than those measured in diffusion experiments.

11.2 Site-specific experimental information

Effects interpreted as surface diffusion in argillaceous media have been observed in compressed bentonite. However, recent laboratory work on samples from the Callovo-Oxfordian at Bure and from the Opalinus Clay in Benken indicate that effective diffusion coefficients for Na exceed those of HTO (Andra 1999 and work in progress at Paul Scherrer Institut, Switzerland).

11.3 Scaling issues

None, because of lack of definition and understanding of process.

11.4 Scientific level of understanding

The level of understanding is poor. The process is invoked to explain differences between measured and predicted diffusion behaviour of cations in compressed bentonite and a small number of argillaceous rocks. The differences may have other causes so that surface diffusion may not actually occur.

11.5 Linked FEPs

FEP 8	Diffusivity
FEP 9	Connected matrix porosity

In addition, sorption properties and the characteristics of double layers considered in the A2.2 series of FEPs are important in evaluating causes for and explanations of surface diffusion.

11.6 Level of understanding from a PA perspective and treatment in PA

Surface diffusion is not explicitly included in PA models. If directly measured diffusion properties (D_a, n_p) are used for PA, the effects of surface diffusion, whether it exists on not, will be included. (See FEP 8).

11.7 Available reviews

Horseman *et al.*, 1996; Lehikoinen, 1999.

11.8 Planned work

None reported.

11.9 Overall evaluation

Understanding of surface diffusion is quite limited, and the process may not occur at all. Most available data refer to compacted bentonite rather than to argillaceous formations, and results are contradictory. The need to invoke surface diffusion can be avoided by using site- and solute-specific diffusion parameters measured by through-diffusion on samples with their *in situ* fabric.

12. COLLOID FORMATION, TRANSPORT AND FILTRATION (FEP A1.3)

12.1 Definition and generalities

Colloids are very fine and well dispersed particles that, in a hydrogeochemical environment, can contribute to the transport of contaminants. Particles of clay minerals, silica, iron oxy-hydroxides, other minerals, organic and bio-organic macromolecules may form the colloid phase. From a size distribution point of view, colloids are defined (IUPAC) as particles with sizes ranging from 1 to 1000 nm.

12.2 Site-specific experimental information

Formation/site	Results and conclusions
Opalinus Clay at Mont Terri	Colloids were studied is several water samples collected *in situ* (Degueldre *et al.*, 1998). Investigations were focussed to the size range 1-10 nm because only such small colloids are potentially mobile in the pore space, and a concentration of 10-20 ppt was derived. Humic colloids are below detection limit.
Opalinus Clay in the Zürcher Weinland	Possible colloids include clay minerals, quartz, calcite, Fe hydroxides and organics, even though their stability under *in situ*-conditions is limited. Mobility of colloids is very low due to the very low permeability and nanometre-scale pore structure of Opalinus Clay. Model calculations indicate that colloid-related transport is negligible (Voegelin & Kretzschmar, 2001). The role of organic colloids in Opalinus Clay is not thoroughly studied. Laboratory experiments indicate that the sorption characteristics of nickel, europium and thorium are independent of the presence or absence of organic colloids (Glaus *et al.*, 2001).
Boom Clay at Mol	Boom Clay acts as an ultrafilter, therefore mobile colloids should only be present in very low concentrations (Ondraf/Niras, 2002).

Only very few studies are available. Colloids that are potentially mobile in the studied argillaceous formations were only found in extremely low concentrations. In many cases, colloid transport is considered irrelevant, at least in cases where fracture flow is not important.

12.3 Scaling issues

None reported.

12.4 Scientific level of understanding

See Section II, Chapter 12.6.

12.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 9	Connected matrix porosity
FEP 15	Natural organics, complexation.
FEP 17	Pore- and fracture water composition
FEP 18	Dissolution / precipitation of solid phases
FEP 20	Ion exchange
FEP 21	Surface complexation
FEP 30	Organics from waste and their effect on transport properties of the host rock

12.6 Level of understanding from a PA perspective and treatment in PA

Colloids, especially in argillaceous systems, are difficult to study. Only very few studies have been performed concerning the behaviour of colloids in argillaceous formations, so the level of scientific understanding is rather low. Actinides are known to form colloids or to associate with colloids. While tetravalent actinides tend to form inorganic colloids, trivalent actinides mainly associate with organic colloids. However, many argillaceous formations are considered to be efficient colloid filters, and colloid-facilitated transport in unfractured media is regarded to be of limited importance. Open points exist in the case of fracture-dominated transport, either in natural fracture systems or in the EDZ.

The effect of colloids on transport in argillaceous formations is regarded as negligible in most PA studies. Conservative estimates can be made by considering a retardation factor R=1 for potentially complexed radionuclides.

12.7 Available reviews

Summary of a working group at NEA's GEOTRAP workshop 2001: Hadermann (2002).

12.8 Planned work

None reported.

12.9 Overall evaluation

This FEP is in general considered not important for unfractured argillaceous formations. It may have some importance in systems with fracture flow.

13. FLOW-WETTED SURFACE AND ACCESSIBILITY OF MATRIX (FEP A2.1.3)

13.1 Definition and generalities

This FEP is of importance mainly in the case of over-consolidated, fractured argillaceous formations. Flow-wetted surface is the surface area per unit rock volume of the walls of fractures where advection takes place. Matrix accessibility refers to the extent to which the rock matrix is accessible by diffusion to solutes migrating through fractures. If fractures, particularly the walls, are mineralised, the accessibility of the rock matrix may be reduced.

13.2 Site-specific experimental information

The most highly indurated sites considered, the Palfris Formation at Wellenberg (Switzerland) and the Boda Clay Formation (Hungary), contain fracture minerals (mostly carbonates), whose distribution is heterogeneous. Permeable structures were observed mainly along the contacts between fracture infill and wall rock, i.e. flowing water is in direct contact with the wall-rock porosity at least at one side. Moreover, even the fracture infills were shown to have a diffusion-accessible porosity (Nagra, 1997).

At the Wellenberg site, only a fraction of all faults penetrated by the boreholes have transmissivity measurable above the detection limit of *ca.* 10^{-9} m^2/s. It was concluded that transmissivity is distributed heterogeneously within each fault (Mazurek *et al.*, 1999), and the possibility exists that not all parts of the fracture surfaces are accessible to flow, which in turn reduces flow-wetted surface.

In the Boda Clay Formation, geological and geochemical indications for water-rock interactions, including mineralogical and isotopic analyses, were investigated in order to identify the locations of past water-flow events (Arkai *et al.*, 2000). Some degree of heterogeneity was observed in the spatial distribution of fracture infills and of the degree of wall-rock alteration (e.g. formation of smectite at the expense of chlorite), indicating that water flow at the time when the water-rock interaction occurred was not distributed evenly, leaving parts of the fractures unaffected.

13.3 Scaling issues

Relevant observations on scales of mm to dm can be made in surface outcrops, tunnels and core materials. This scale is the same as the one required for the conceptualisation of migration pathways for transport calculations.

13.4 Scientific level of understanding

Indications exist that the distribution of flow in faults and fractures in indurated shale formations is heterogeneous. Therefore, flow-wetted surface may be smaller than the total area of fracture walls per unit volume. Data and approaches pertinent to fractured argillaceous systems are limited at present. Approaches to estimate and conceptualise flow-wetted surface are well developed in PA programmes targeted at crystalline rocks, e.g. in Sweden or in Finland.

13.5 Linked FEPs

FEP 1	Advection/dispersion
FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 16	Mineral-surface area
FEP 18	Dissolution / precipitation of solid phases
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 41	Swelling
FEP 42	Self-sealing
FEP 53	Past deformation events
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

13.6 Level of understanding from a PA perspective and treatment in PA

This FEP is important only in highly indurated formations where fracture flow dominates. The only example of PA treatment comes from the Palfris Formation at Wellenberg (Switzerland), where flow-wetted surface was derived directly from cm- to dm-scale geometric conceptual models of the migration pathways (Nagra, 1997).

13.7 Available reviews

None reported.

13.8 Planned work

None reported.

13.9 Overall evaluation

Flow-wetted surface is a parameter related exclusively to indurated shale formations where fracture flow is important. It is of no concern in diffusion-dominated systems. There are no indications of limited matrix accessibility. Fracture infills themselves are porous, and in general at least one side of a fracture is in direct contact with the rock matrix.

Heterogeneity of fractures may result in a reduction of flow-wetted surface. Given the fact that matrix diffusion in argillaceous formations can be regarded as unlimited, large matrix volumes of rock can be accessed by diffusion even if the areas of contact with flowing water are limited.

14. LITHOLOGY, MINERALOGY OF ROCKS AND FRACTURE INFILLS (FEP A2.2.1)

14.1 Definition and generalities

Lithology and mineralogy of rocks and fracture infills affect the hydrogeological, chemical transport, geomechanical and other properties of the formation. The electro-chemical behaviour of minerals is of prime importance for sorption processes. Mineralogy also determines the chemistry of the ground water through a range of bulk water-rock interaction processes and related mechanisms such as osmotic processes, diffusion and matrix diffusion.

The occurrence of fractures may differ from one type of argillaceous formation to another. In well-consolidated shales, fractures are common and they are often filled with secondary minerals. In contrast, in plastic clays, fractures are less common and contain less or no infill material.

14.2 Site-specific experimental information

Formation/ site	Type of information	Results and conclusions
Callovo-Oxfordian at Bure	Deep boreholes, geophysical logs, 2-D seismics, 3-D seismic survey, logs from petroleum drillings in the region	The host rock consists of three sedimentary sequences, which correspond to marine depositional cycles and result in different lithologic facies (from bottom to top): • 555-520 m below surface: 35 m thick homogeneous silty shales (C2a facies) of Callovian age, directly overlying Dogger carbonates. • 520-440 m below surface (Oxfordian): a. 45 m thick, homogeneous shaly member (C2b1 facies), starting with a six metres thick layer including five decimetric sections of shaly limestones. The clay-mineral content progressively increases to 50 - 60% up to 495 m depth and stays high until 475 m below surface. b. 16 m thick sequence of silty and carbonaceous shales (C2b2 facies) showing a smooth decrease of clay-mineral content. c. 19 m thick sequence of shaly, carbonaceous siltstone (C2c facies), showing a major a decrease of clay-mineral content and an increase of quartz and carbonates at the top of the interval. • 440 to 422 m below surface: 18 metre thick sequence of carbonaceous silt of Oxfordian age (silty and dolomitic biomicrite - biosparite. Clay-mineral content progressively increases to the top. The top of this lithologic facies, also highlighted by a distinct level in many geophysical logs, is considered as the top of the host formation. On the average, the Callovo-Oxfordian shales contain 40 to 45% clay minerals. An interstratified illite-smectite phase is the most abundant clay mineral, with the “R1” type (60 to 75% of illite in the mixed-layer phase) in the lower part and the “R0” type (40 to 60% of illite) in the upper part. The progression from “R1” to “R0” takes place in a 10 m thick interval at around 495 m below surface. To date, no fractures have been identified in the host rock.

Formation/ site	**Type of information**	**Results and conclusions**
Toarcian-Domerian at Tournemire	Underground research laboratory, boreholes	The mineralogy of the Toarcian shales and marls is characterised by a predominant clay fraction (40-50%) (mica, kaolinite, illite and illite/smectite mixed layers with more than 70% of illite). Calcite is the predominant carbonate. Muscovite, biotite, albite and K-feldspar have been identified by scanning electron microscopy. Framboïdal pyrite and organic matter are widespread (Boisson *et al.*, 1998). Fracture mineralogy includes calcite, cubic pyrite and trapped matrix pieces in minute amounts. The scale of fractures ranges from microscopic to major faults with breccia and crushed material. Some fractures are characterised by geodic cavities related to fault-plane displacements (Mathieu, 1999, Mathieu *et al.*, 2000).
Spanish Reference Clay in a Tertiary basin	Deep boreholes, geophysical logs, 2-D seismics	The formation consists of plastic, rather massive lacustrine argillaceous sediments with sandy admixtures and intercalations of gypsum and anhydrite. The average mineralogy is dominated by clay minerals (*ca.* 80%, mainly smectite, illite ± chlorite, kaolinite), calcite (*ca.* 12%) and minor quartz, dolomite and gypsum.
Opalinus Clay in the Zürcher Weinland	Deep borehole	The Opalinus Clay can be subdivided stratigraphically into 5 sub-units, which can be correlated regionally. The lithological variations in the vertical (and in the horizontal) direction are minor. The lower 2 sub-units (*ca.* 22 m thick) are very rich in clay minerals (>60%), whereas the upper 3 units contain more quartz and less clay minerals (40-60%) and are slightly more heterogeneous on a scale of cm-dm. The average mineralogy in the Benken borehole (Nagra, 2001) consists of 53% clay minerals (illite, illite/smectite mixed-layers, kaolinite, chlorite), 21% carbonates (calcite ± dolomite/ankerite, siderite) and 20% quartz. Accessories include feldspars, pyrite and organic matter. Fracture infills are very rare and volumetrically insignificant. They include calcite, baryte, celestite and quartz.
Opalinus Clay at Mont Terri	Underground research laboratory, boreholes	Lithology and mineralogy are very similar to those of the Benken borehole, and the vertical subdivision is also very similar (Thury & Bossart 1999, Nagra 2002). The biggest difference is the occurrence of a sandy-calcareous sub-unit at Mont Terri, which contains more quartz (*ca.* 25%) and calcite (*ca.* 35%) at the expense of clay minerals (*ca.* 30%). In spite of the substantial deformation of Opalinus Clay at Mont Terri, fracture mineralisations are very rare and include the same minerals as in the Benken borehole.

Formation/ site	Type of information	Results and conclusions
Boom Clay at Mol	Underground research laboratory, boreholes, surface outcrops	The Boom Clay at Mol consists of a rhythmic alternation of silty clay and clayey silt with increasing silt content at the base and at the top. It is most homogeneous in the central part. Septarian carbonate concretions are the most relevant lithological heterogeneities (dm scale). Mineralogy includes clay minerals (*ca.* 60%, illite, smectite, kaolinite, illite/smectite mixed-layers, ± chlorite, glauconite), quartz (*ca.* 20%) and feldspars (*ca.* 10%). Accessories include calcite, pyrite and organic matter. References: Griffault *et al.* (1996) (Mol site), Vandenberghe (1978) (sedimentology, granulometry, mineralogy, geochemistry in clay pits of northern Belgium), Vandenberghe *et al.* (1998) (sedimentary cycles), Van den Bosch & Hager (1984) (lithology and lithostratigraphic correlation in boreholes in the North Sea, northern Belgium, the Netherlands and Germany).
Boda Clay Formation at Mecsek	Underground research laboratory, deep boreholes, surface outcrops	The formation originates from lacustrine sediments deposited under oxidising and alkaline conditions. The main lithology are albitic claystones. The formation was buried to 3.5-4.5 km below surface and so is highly indurated. It contains fractures and faults originating from a number of tectonic events. It can be subdivided into three sequences: • Transitional beds from the underlying formation, predominantly brown, reddish brown sandstone with high mica content and ripple marks, and brown siltstone, green shale and limestone interbeds (100-150 m thick). • Reddish brown, albitic shale with cross-bedded siltstone and sandstone layers with calcite and albite as cements, with ripple marks and mica-bearing bedding planes, and sometimes dolomite interbeds. • Reddish brown albitic, silty shale containing dolomite interbeds and dolomite concretions with desiccation cracks. In this part max. 2-3 m thick, dark grey, black, albitic, pyrite-bearing shale interbeds occur (reduced layer containing organic material). The mineralogical composition includes authigenic albite (12-59%), illite-muscovite (7-45%), clastic quartz (2-33%), chlorite (0-18%), hematite (5-10%), dolomite, calcite (5-10%; higher in calcareous interbeds). Accessory clastic components include K-feldspar, plagioclase, biotite, muscovite, chlorite, apatite, zircon, rutile, Fe-Ti oxides. A small fraction of samples contains chlorite/smectite, illite/smectite mixed-layer minerals and/or discrete smectite, vermiculite, kaolinite and traces of siderite, anhydrite, gypsum, barite, authigenous K-feldspar and sulphides of chalcophilic elements (galenite, chalcopyrite, sphalerite). Reduced interbeds contain pyrite and organic matter.

Formation/ site	Type of information	Results and conclusions
Boda Clay Formation at Mecsek	Underground research laboratory, deep boreholes, surface outcrops	On the basis of the relative proportions of the major mineral constituents, the following lithological units can be defined: • Albitic shale (most abundant). • Albitolite (rock type with an albite content >50%). • Siltstone. • Dolomite. • Sandstone. Fracture infills can be classified as follows: 1. Tectonic zones filled with fault rocks, whose mineralogy is mostly identical to the one of the adjacent wall rocks. Sometimes a limited amount of smectite formed at the expense of chlorite. 2. The most frequent group of infillings consists of calcite veins with traces of quartz, barite and dolomite. The textural observations suggest a multi-stage evolution of the veins. 3. Vein-mineral association dominated by barite-quartz, with admixtures of calcite (always present), dolomite, albite and traces of chlorite, anhydrite, Cu-sulphides (chalcopyrite, bornite, covelline). This mineral association suggests a low-temperature hydrothermal origin (about 150°C). 4. Veins dominated by anhydrite, accompanied by calcite and albite. Albite always constitutes a thin rim between the rock and the anhydrite vein. This vein type is characteristic for the lower part of the formation.

Formation/ site	Type of information	Results and conclusions
Diverse argillaceous formations in UK		A large number of argillaceous formations was studied: Tertiary London Clay, Upper Jurassic (Kimmeridge Clay, Oxford Clay) and Lower Jurassic (Lower Lias Clays) and also Quaternary sediments (boulder clay) (see Bloodworth & Morgan, 1989). Additional information includes Permo-Triassic samples (Eden Shale, St Bees Shale) and Devonian samples (Caithness Flagstones). The regional data coming from all over the UK provide information on the variation of clay mineralogy with geological age. The proportion of illite and chlorite increases with age, with a corresponding decrease in levels of kaolinite and expandable clay minerals. The nature of the expandable clay minerals changes from predominantly smectite in the Tertiary to mixed-layer clay minerals in the Mesozoic and Palaeozoic. These trends are similar to those expected with increasing levels of burial diagenesis. The dominance of smectite, occasionally associated with zeolites, in the London Clay reflects the significant volcanic input to sediments at that time. Distinctive clay-mineral assemblages in Permo-Triassic shales, including sepiolite, palygorskite and smectite/mixed layer clay minerals reflect the highly saline pore-water conditions during deposition and early diagenesis at that time.

14.3 Scaling issues

Information obtained is typically at microscopic to drillcore scale, whereas the scale needed for PA is from tens to upwards of hundreds of metres. Upscaling requires techniques to deal with possible heterogeneity in lithological organisation, mineralogical composition and nature of fracturing. Relevant information can be obtained from outcrops, other boreholes in the region, and seismic data.

14.4 Scientific level of understanding

Lithology and mineralogy of rocks and fracture fillings are well understood parameters. Heterogeneity in the vertical dimension is generally well known due to the availability of borehole-derived information. In the horizontal dimensions, the evidence is mostly indirect and based on interpolation to other boreholes/outcrops in the region or on seismic data.

As an example, it is well-known that variations in grain size (alternation silty clay – clayey silt), organic matter contents (black beds), and carbonate contents (calcareous layers with carbonate concretions) are present in the Boom Clay, resulting in the typical layering of the deposit (Vandenberghe 1978). Some layers may differ from the average composition, for example the calcareous layers contain about 15% carbonate while the average carbonate content is only a few %.

14.5 Linked FEPs

FEP 18	Dissolution/precipitation of solid phases
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 50	Past burial history

14.6 Level of understanding from a PA perspective and treatment in PA

Lithology affects both transport (advection, diffusion) and retention (matrix diffusion, sorption) properties of the rocks. In general, both vertical and large-scale lateral lithological variations are sufficiently well known for PA purposes. One possible exception are sites that had been subjected to intense thrusting and imbrication, such as the Wellenberg in the Swiss Alps, where the spatial distribution of lithologies is more difficult to determine and needs to consider several datasets (boreholes, seismics, regional tectonics).

Lithology and mineralogy are not used in PA models as explicit parameters. They are considered indirectly in several other parameters to which they are connected, e.g. sorption K_d, porosity, diffusion coefficient, permeability, geomechanical parameters. While some programmes consider averaged parameter values for the whole host-rock formation, others use different parameter sets for different lithological units within the formation.

Mineralisations in fractures and faults occur in indurated formations and, in general, are not included in PA calculations. The most important question to answer is whether or not fracture coatings could isolate flowing water from the matrix.

14.7 Available reviews

None reported.

14.8 Planned work

Boom Clay at Mol:

- Study of the long-term behaviour of natural trace elements and radionuclides in layers with different lithological characteristics (silty clay, clayey silt, carbonate-rich, organic matter containing).
- Uranium migration experiments in layers with different lithological characteristics (silty clay, clayey silt, carbonate-rich, organic matter containing).
- It is planned to account for heterogeneity (layering) of the host formation in the PA calculations.

Nirex (generic studies):

- Programme of laboratory experiments on relating sorption parameters to individual mineral phases and a range of rock types. The objectives are to improve the data base of parameters applied to sorption modelling.
- Application of geophysical techniques, especially borehole electrical conductivity, to characterising lithological and mineralogical properties relevant to sorption and other retardation processes (including diffusion).

14.9 Overall evaluation

Lithology and mineralogy are among the best known properties of the host formations, and in most cases conceptual models for the large-scale spatial distribution of lithologies are well developed. The heterogeneous architecture of the host formation is treated explicitly in some PAs. Fracture fillings are generally well characterised and play a minor role from a PA perspective.

15. NATURAL ORGANICS, COMPLEXATION (FEP A2.2.2)

15.1 Definition and generalities

The term “natural organics” refers to the plethora of structurally different organic molecules present in the geosphere. They are formed by decay and cycling processes from plant, microbial and animal materials. They can be subdivided into carbohydrates, lipids, amino acids/proteins and humic substances (HS), just to mention a few important classes. With respect to PA, the term “natural organics” is most often restricted to humic substances, because these are among the most important complexing agents and are ubiquitously present in ground water. Humic substances are part of an operationally defined class of structurally related molecules. They are mixtures of macromolecular organic structures, their functional groups being to a large extent carboxylic and phenolic. The soluble part of humic substances is further subdivided into humic and fulvic acids.

Organic carbon in water is generally measured by analysing the quantity of CO_2 produced when a water sample is oxidised. The results are expressed as TOC (total organic carbon) or DOC (dissolved organic carbon) concentrations. TOC measurements are made on samples as collected; DOC measurements are made on samples after filtration.

15.2 Site-specific experimental information

Humic substances are ubiquitously present in geological fluids at low concentrations of the order of a few µg/l up to hundreds of mg/l (Grauer, 1989). They may increase the mobility of radionuclides due to complexation, and they may induce changes of the redox state. Conclusions from natural analogue and field studies with respect to the influence of humic substances on the mobility of radionuclides are conflicting. An overview can be found in Choppin (1992). One example showing an increase in Cu(II) concentrations induced through increased humic-substance concentrations is given by Lehman & Mills (1994). Organic matter can also be present in an immobile state (insoluble or ultrafiltered by the argillaceous rock). This immobile organic matter can have a high sorption capacity for the radionuclides and thus contributes considerably to the retention of radionuclides (Dierckx *et al.*, 2000).

Formation/ site	Type of information	Results and conclusions
Callovo-Oxfordian at Bure	Analysis of cores	0.5 to 1% organic carbon in the rock, immature.
Toarcian-Domerian at Tournemire	Analysis of cores	Up to 1% organic carbon in the rock, very mature (Boisson *et al.*, 1998); low complexation.

Formation/ site	**Type of information**	**Results and conclusions**
Spanish Reference Clay in a Tertiary basin	Complete chemical analysis of pore-water but no data on dissolved organic matter	Not well studied at present. Included in PA through uncertainty ranges of solubilities (Enresa, 1999).
Opalinus Clay in the Zürcher Weinland and at Mont Terri	Aqueous extracts; sorption tests on natural organics in Opalinus Clay with Ni(II), Eu(III) and Th(IV) and complexation tests with Cm(III); complexation studies with humic substances	DOC ~5 to 15 mg/l. Sorption of Ni(II), Eu(III) and Th(IV) on an ion-exchange resin was studied using 1) synthetic pore-water and 2) aqueous extracts of three samples of Opalinus Clay from Mont Terri and three samples from the Benken borehole. When using the aqueous extracts, a slight reduction (less than half an order of magnitude) of sorption on the resin was observed when compared to the synthetic pore-waters. Thus sorption on dissolved organic matter that is present in the extracts was shown to be of limited significance. Experiments using small molecular weight ligands and Aldrich humic acid show that the sensitivity of the ion exchange method is sufficient at the specific conditions of the Opalinus Clay extracts. The results of the accompanying fluorescent spectroscopic test experiments using Cm(III) as a fluorescent probe do not show any influence of the extracts on metal ion speciation, which is dominated by carbonate complexes. This indicates that the reduction of sorption observed in the ion exchange experiments is possibly not caused by formation of complexes between the radionuclides and the dissolved organic matter in the extracts, but is rather due to slight differences in the chemical matrix (i.e. water chemistry) between the extracts and the synthetic reference waters. From these findings and from a rough characterisation of the dissolved organic matter in the extracts by UV-VIS spectroscopy, it can be concluded that only a negligible fraction of the dissolved organic matter may be present as humic or fulvic material. The largest part of the dissolved organic matter are most probably either small molecular weight organic molecules or organic macromolecules with a very low content in complexing ligand sites. The measurement of sorption distribution coefficients will not be affected by the extractable organic matter contained in Opalinus Clay. The samples of Opalinus Clay tested can be considered to be representative for the formation at Mont Terri and in the Zürcher Weinland. The conclusions drawn here for organic matter obtained from samples at Mont Terri can safely be conferred to the Opalinus Clay in the Zürcher Weinland

Formation/ site	Type of information	Results and conclusions
		SUMMARY: Dissolved organic matter has only very low content in complexing ligand sites, with little influence on sorption (Glaus *et al.*, 2001). Complexation studies were also performed with pure humic substances (i.e. artificial materials, not derived from Opalinus Clay). These are considered to be the most strongly complexing organic materials and so represent the "worst case". Opalinus Clay is poor in humic substances. Strong complexation of humic substances exists towards a series of radionuclides, such as transition metals, lanthanides and actinides (Grauer, 1989, Glaus *et al.*, 1997, 2000, Hummel *et al.* 2000). From all the safety relevant radionuclides, trivalent actinide ions, such as Am(III), Cm(III), are most strongly affected by the presence of humic substances (Glaus *et al.*, 1997, Hummel *et al.*, 2000). The stability of metal-humate complexes generally increases with increasing pH and increasing ratio of humic substance to metal ion concentration (Glaus *et al.*, 1997, Hummel *et al.* 1999, 2000). The stability of these complexes is rather weakly influenced by changes in ionic strength and in variation of type of the humic substance (with respect to origin and subdivision in humic and fulvic acids).
Boom Clay at Mol	Analysis of clay cores, analysis of pore-waters, charge measurements, complexation studies, laboratory and *in situ* migration studies	The total organic matter content of Boom Clay ranges from 1 to 3 wt%. Only a small fraction is soluble and mobile. TOC contents are 40 to 250 ppm (mean 100 ppm). From U/Th series disequilibrium studies on Boom Clay (De Craen *et al.*, 1999, 2000), an association was observed between U and solid organic matter. This association was also observed in a study using different extraction techniques to determine the natural U content in Boom Clay (Wang *et al.*, 2001, 2002), but the type of interaction remains unknown. More detailed studies on the complexation behaviour of U with dissolved organic matter are undertaken in the EC-project TRANCOM-II: complexation experiments (batch) and column experiments (migration experiments). Batch experiments in the laboratory: A complexation study was carried out for trivalent lanthanides (Eu^{3+}) and actinides (Am^{3+}) with organic matter extracted from Boom Clay at *in situ* pH (around 8) and in presence of the *in situ* concentration of carbonate, and complexation constants were derived (Dierckx *et al.*, 1994; Maes *et al.*, 1988, 1991). In more recent batch experiments (Trancom-Clay, Trancom-II), the organic matter for the complexation experiments is taken from Boom Clay pore-water sampled in the underground research lab and then concentrated.

Formation/ site	**Type of information**	**Results and conclusions**
		Column experiments in the laboratory: Site specific organic material was labelled with ^{14}C and contacted with ^{241}Am to form Am complexes. Based on the conditional complexation constants from batch experiments, the speciation was predicted to be entirely an organic matter complex. The main result was that upon passage through the clay, the complex dissociates and that during percolation through real clay water, a rather constant but tiny concentration (10^{-14} to 10^{-11} M) was leached from the clay core (Dierckx *et al.*, 2000). The conditional complexation constant for trivalent radionuclide complexation in solution has been implemented in the CHESS data base (Van der Lee, 1998). Based on conditional complexation constants for trivalent radionuclide complexation in solution, the distribution of americium in the clay environment between solid and solution was predicted. The americium is said to be quantitatively sorbed (Dierckx *et al.*, 2000).
Boda Clay Formation at Mecsek	Analysis of cores	Almost no organic matter in shale due to oxidising conditions during sedimentation and diagenesis. Any remaining organics would be highly mature. Organic matter only present in over- and underlying aquifers.
Mizunami Group at Tono	Chemical analysis of water from boreholes	DOC 0.1 to 8 mg/l. Trace elements such as I, Cs, Th, Cr and REE are not identified in fulvic and humic acids, i.e. they are not sorbed. Some sorption is identified for Cu and Mn (Iwatsuki & Yoshida, 1999).

15.3 Scaling issues

Information about the nature of dissolved organics and their complexation with metal ions is restricted to the laboratory scale. With respect to *in situ* conditions, these data are often conservative because conservative assumptions are made in the evaluation and modelling of the laboratory experiments (e.g. Glaus *et al.*, 1997, Hummel, 1997, Hummel *et al.*, 2000).

15.4 Scientific level of understanding

The various interactions between humic substances, ions and the solid surface are complex and not fully understood. Humic substances are known to complex especially trivalent actinides. There is no consensus on how to treat metal-humate interactions in a consistent way, and these interactions cannot be described using simple thermodynamic equilibrium expressions. The ligands, i.e. humic substances, are not well characterised chemical structures. They are rather an operationally defined mixture of naturally occurring medium and large size molecules. The mixture is heterogeneously composed both in the sense of molecular size and of functional groups. Therefore, the interactions are currently mostly described using conditional constants or empirical relationships. There are only few studies on the migration of humic-substance complexes in argillaceous formations, and so the mobility/immobility and stability of these complexes is poorly understood.

In Boom Clay at Mol, knowledge is thought to be adequate for trivalent radionuclides (Am, Cm, Pu). For other critical radionuclides, the fitted R (K_d) value lumps complexation with immobile organic matter together with other mechanisms such as surface complexation, and so it can be incorporated into the R (K_d) value. It is necessary to study the FEP in detail for system understanding.

15.5 Linked FEPs

FEP 14 Lithology, mineralogy of rocks and fracture infills

FEP 17 Pore- and fracture water composition

FEP 21 Surface complexation

FEP 22 Thermodynamic and kinetic modelling data: *The "blind use" of humic-substance complexation data in thermodynamic data bases is dangerous. Problems may arise when extrapolating data measured under ideal laboratory conditions (i.e. low pH, large metal ion concentrations) to repository relevant conditions (over-optimistic).*

FEP 26 Oxidation of the host rock

FEP 27 Redox buffering capacity of the host rock

FEP 30 Organics from waste and their effect on transport properties of the host rock: *Other ligands transported from the affected field to far field may also be of importance. The identification of the dominant ligand in a mixture of natural and artificial organic substances with respect to radionuclide complexation is an important task and has to be based both on effective solution concentration of the ligand and on its complexing strength (direction unclear).*

FEP 31 Thermal effects on mineral stability and pore-water composition

FEP 50 Past burial history

15.6 Level of understanding from a PA perspective and treatment in PA

The current level of understanding is sufficient in some programmes (e.g. Belgium, Switzerland) to allow conservative estimates of the effect of natural organics on repository performance. Complexation with natural organics is, where relevant, treated in a conservative way in PA, either implicitly by using adapted uncertainty ranges for e.g. solubility (e.g. Spain), "operational" solubility (e.g. Belgium) or, as in Switzerland, explicitly by applying a "conservative roof" model.

The Swiss "conservative roof" model (Glaus *et al.*, 1997, Hummel 1997; Hummel *et al.*, 2000) is an empirical approach to describe the overall effect of humic substances on the speciation of radionuclides, and it has been specifically developed for the purposes of PA. It is based on a consistent treatment of own measurements (Glaus *et al.*, 1997, Glaus *et al.*, 2000) and of a broad variety of traceable (!) literature data. It uses empirical relationships (not deduced in a deterministic way from thermodynamic principles) to model the interaction between metal ions and humic substances. Consequently the applicability of the model – especially with respect to pH, metal concentration, ionic strength – is restricted to the parameter space within which the experimental data have been obtained.

However, this parameter space has been chosen such as to meet the needs of PA. The model reduces noticeably the various features (i.e. metal concentration effect, pH effect, ternary complexes, organic coating, ionic strength, competition by anions or cations, sorption), in the sense that it only comprises the ones that lead to an increase of the radionuclide concentration in solution. The complexation constants can be used in a generic way, i.e. they do not depend on the type of humic substance.

A simplified treatment is used for Boom Clay at Mol. For trivalent radionuclides, the concept of “operational solubility” is used to describe the small mobile fraction (Dierckx *et al.*, 2000). For other critical radionuclides, the distribution between the solid and the solution is treated within a K_d concept. Calculations with conservative parameters are performed to try to estimate the maximum impact of organic complexation.

15.7 Available reviews

Swiss site-specific studies on quantification of natural organic matter and on complexing effects of organic matter extracted from argillaceous formations: Tits *et al.* (1993), Lauber *et al.* (1998, 2000).

Boom Clay: Dierckx *et al.* (2000).

Literature overview and identification of PA-related needs for research: Grauer (1989). Generic work on complexation of a series of radionuclides by humic substances: Glaus *et al.* (1997, 2000), Hummel (1997), Hummel *et al.* (2000).

General overview: De Cannière *et al.* (1996).

Belgian work published in the scientific literature: Dierckx *et al.* (1998), Put *et al.* (1998).

15.8 Planned work

Both in Switzerland and Belgium further studies are planned. These studies will be oriented to a better treatment of this FEP in PA.

The question of the actual concentration of dissolved humic substances in deep Swiss ground water is not yet settled. Just taking dissolved organic C values as representative for the concentration of humic substances may grossly overestimate their influence. Site specific work aiming at determining the overall effect of complexation of extractable natural organic matter towards selected radionuclides (without a detailed characterisation of the organic matter) is ongoing (Lauber *et al.*, 2000). There is not yet any experimental confirmation for the estimated equilibrium constants for the complexation of tetravalent actinides by humic substances available. A short study determining a few key points using the equilibrium dialysis ligand exchange method (Van Loon *et al.*, 1992) would therefore be desirable.

A large-scale diffusion experiment with ^{14}C labelled site-specific organic material is running in Boom Clay at Mol. The objective of this experiment is to confirm the laboratory results. No conclusions are drawn yet and modelling is foreseen in the near future.

15.9 Overall evaluation

This FEP is relevant for argillaceous formations containing natural organics (especially immature). Although conservative data and/or models were used, the effect of natural organics on the performance of a multi-barrier system was found to be small and limited to migration of trivalent actinides.

16. MINERAL-SURFACE AREA (FEP A2.2.3)

16.1 Definition and generalities

The specific surface area of a mineral or rock is the amount of reactive surface area available for adsorbing solutes per unit weight of the material. The surface area available for sorption can be solute dependent (internal/external surface areas, anion exclusion). Total surface area is the sum of the external and internal surfaces, the latter being the area of interlayers in smectite. External surfaces can be measured by adsorption of non-polar substances, such as N_2. Total surfaces are measured by adsorption of polar molecules, such as H_2O or ethylene glycol. Internal surfaces are calculated by difference.

16.2 Site-specific experimental information

Formation/ site	Type of information	Results and conclusions
Callovo-Oxfordian at Bure	N_2-BET measurements	30 m^2/g (external surface)
Toarcian-Domerian at Tournemire	N_2-BET measurements	23-29 m^2/g (external surface) (Boisson *et al.*, 1998)
Spanish Reference Clay in a Tertiary basin	N_2-BET measurements	41-65 m^2/g (external surface)
Opalinus Clay at Mont Terri (Nagra 2002)	N_2-BET measurements on crushed and intact samples	24-37 m^2/g (external surface) (Bradbury & Baeyens, 1998b)
	Ethylene-glycol measurements on small samples	100-220 m^2/g (total surface)
	H_2O isotherms	112-147 m^2/g (total surface)
Opalinus Clay in the Zürcher Weinland (Nagra 2002)	N_2-BET measurements	23-34 m^2/g (external surface)
	EGME measurements, H_2O isotherms	56-107 m^2/g (total surface)

Formation/ site	Type of information	Results and conclusions
Boom Clay at Mol	N_2-BET measurements on representative sample of a large volume of crushed Boom Clay taken from the underground research laboratory	44 m^2/g (external surface) (Volckaert & Vandervoort, 1992)
	Ethylene-glycol measurements	200-250 m^2/g (total surface) (Baeyens *et al.*, 1985)
Palfris Formation at Wellenberg	N_2-BET measurements	2-12 m^2/g, average 7 m^2/g (external surface) (Mazurek *et al.*, 1994)

A trend of decreasing internal and external surface areas can be seen with increasing induration, which reflects recrystallisation and the decrease of smectite (or smectite layers in an interlayer phase) with increasing temperature during diagenesis.

16.3 Scaling issues

Only small-scale (cm) measurements are available, and the representativity of the measurements over the whole formation can be based on the correlation with the mineralogical composition. An additional point is the fact that most measurements were made on crushed samples, and the possibility of creating artificial surfaces during crushing needs to be addressed.

16.4 Scientific level of understanding

The theory and standard techniques behind surface-area measurements are generally well understood and data for many minerals and rocks are available in open literature. However, the understanding of these surface areas in relation to *in situ* migration and sorption is rather poor. Because of the measurement methodology, surface-area measurements can only be regarded a rough estimates of the surface areas available *in situ*. They may be useful for providing relative values for systems with different mineralogy.

16.5 Linked FEPs

FEP 14 Lithology, mineralogy of rocks and fracture infills

FEP 18 Dissolution/precipitation of solid phases

FEP 24 Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units

FEP 29 Interactions of hyperalkaline fluids and host rock

16.6 Level of understanding from a PA perspective and treatment in PA

The mineral surface area is not directly used in PA models. However, it is required by surface complexation models that could be used as models supporting PA. For this purpose, the degree of knowledge about surface area is regarded as sufficient.

16.7 Available reviews

Davis & Kent (1990), Van Olphen (1970).

16.8 Planned work

None reported.

16.9 Overall evaluation

This FEP is currently not directly treated in PA but is a necessary supporting parameter, e.g. for the extrapolation of laboratory sorption data to *in situ* values.

17. PORE- AND FRACTURE-WATER COMPOSITION (FEP A2.2.4)

17.1 Definition and generalities

The pore and fracture water composition includes the concentrations of dissolved solids and gases and of suspended solids, the values of such geochemically significant properties as pH, temperature and redox potential and the isotopic composition of water and its solutes. These data are used in both site characterisation and PA activities. They are relevant to the far field in connection with site characterisation and nuclide transport properties for PA and to the affected field as boundary conditions for analysis of the engineered barrier system.

The composition of water flowing in fractures is distinguished from that in the matrix of argillaceous rock. The matrix water is further subdivided into *bound* water, which is sorbed to or structurally influenced by charged clay-mineral surfaces and edges, and *free* water, which is present in the open pores of the rock. Fracture water can be sampled from conventional, surface-drilled boreholes. Matrix pore-water does not flow into such boreholes but several other techniques are available for its characterisation. The terminology of pore-water sample types is not standard in the literature nor among waste management organisations. The definitions developed in the Mont Terri Project (Pearson *et al.*, 2003) are adopted here.

The *in situ* pore-water chemistry is that of the free pore-water as it exists in the rock. Water samples collected from sub-surface boreholes or piezometers represent *in situ* pore-water and have successfully been collected from the Opalinus Clay at Mont Terri with hydraulic conductivity below 10^{-12} m/s, and from the Boom Clay at Mol with hydraulic conductivity below 10^{-11} m/s. Values for such properties as the pH, redox potential and gas partial pressures may change during borehole sampling, but *in situ* values may be recoverable by geochemical modelling. Samples squeezed from core at high pressures or by high-speed centrifugation also represent pore-water, but are subject to many perturbations such as oxidation and gas exchange during core collection, storage, preparation and squeezing. Very high pressure squeezing may also result in different salinity and ion ratios than in the *in situ* pore-water because of ion filtration and perhaps pressure solution of minerals resulting from the changing pore geometry with increasing pressure. The Cl^- contents of samples squeezed from Opalinus Clay core from Mont Terri had the same Cl^- content as samples from subsurface boreholes when squeezed at pressures up to 200 MPa, but 25% lower Cl^- contents when squeezed at 512 MPa (Pearson *et al.*, 2003, Annex 2).

The isotopic composition of matrix pore-water in a core can be measured on samples extracted by distillation or by an isotopic exchange procedure. The concentration of readily soluble salts per mass of core material can be determined by aqueous leaching techniques. These are subject to the same artefacts as samples obtained by squeezing and to additional reactions such as mineral dissolution and cation exchange during the leaching process. To convert salt contents per mass rock to concentrations per mass water requires knowledge of the geochemical or free water porosity (see FEP 9). Sampling methodology has recently been reviewed by Sacchi & Michelot (2000), and the techniques used at Mont Terri are described and evaluated by Pearson *et al.* (2003).

17.2 Site-specific experimental information

Formation/site	Water type	Characterised by	Water chemistry
Callovo-Oxfordian at Bure (Andra 1999a)	Matrix	Boreholes; core squeezing, core leaching	Data based on squeezing: Total dissolved solids (TDS) 2.7 - 8.5 g/l, Cl 0.7 - 2 g/l; waters dominated by Na and Cl (possibly also SO_4). Cl values based on aqueous leaching are similar to the ones above when assuming that Cl-accessible porosity is about half of total porosity.
Toarcian-Domerian at Tournemire (De Windt *et al.* 1997, 1998, 1999, Moreau-Le Golvan *et al.* 1998)	Fracture	Boreholes	Adjacent shallow ground waters: Ca-HCO_3, *ca.* 0.2 mM Cl, pH *ca.* 7.5. Fractures within the argillaceous host formation: Na-Cl-HCO_3, *ca.* 10 mM Cl, pH *ca.* 8.
	Matrix	Core leaching, modelling	Na-Cl, *ca.* 20 mM Cl, pH 7.4 (assumed).
Spanish Reference Clay in a Tertiary basin (Turrero *et al.* 2001, Ciemat 1999)	Matrix	Boreholes; core squeezing, core leaching, modelling	Na-SO_4, ionic strength = 0.24 mol/l (0.12 - 0.29).
Opalinus Clay and Liassic shales at Mont Terri (Pearson *et al.* 2003)	Matrix	Subsurface boreholes and *in situ* measurements; core squeezing; core leaching; core distillation and exchange; modelling	Na-SO_4-Cl, Cl from 0.3 M at Liassic/Opalinus-Clay contact to < 0.05 M Cl at bounding Dogger and Keuper limestones. He, H_2O isotopes, Cl show a diffusion profile.
Opalinus Clay in the Zürcher Weinland (Nagra 2002)	Matrix	Core squeezing; core leaching; core distillation and exchange; modelling	Na-SO_4-Cl, Cl from 0.2 M at top of Opalinus Clay and in overlying Dogger to < 0.05 M at bounding Keuper limestone.
Boom Clay at Mol (Henrion *et al.* 1985, Griffault *et al.* 1996, Dierckx 1997)	Matrix	Subsurface boreholes and *in situ* measurements; core squeezing; core leaching; modelling	12.5 mM Na-HCO_3; pH 8.0 to 8.5; reducing (-250 to -400 mv SHE).

Formation/site	Water type	Characterised by	Water chemistry
Boda Clay Formation at Mecsek	Fracture	Surface and subsurface boreholes	Shallow waters in the Boda Clay Formation: $Ca\text{-}Mg\text{-}HCO_3\text{-}SO_4$, local meteoric water. Subsurface-sampled waters: $Na\text{-}HCO_3\text{-}SO_4$, TDS 1.5 – 7 g/l.
Palfris Formation at Wellenberg (Nagra 1997, Pearson *et al.* 1998)	Fracture	Surface boreholes; sample chemistry corrected for contamination; chemical evolution and mixing modelled	< *ca.* 70 m: < 70 a, oxidising $Ca\text{-}HCO_3$, low Cl, local meteoric water. *ca.* 70 – *c.* 400 m: < 10-15 ka, $Na\text{-}HCO_3$, low Cl local meteoric water. > *ca.* 400 m: Na-Cl, to 0.2 M Cl, resembles fluid inclusions from last Alpine metamorphism.
Various argillaceous formations in UK (Bath 2001)	Matrix	Core squeezing; core leaching; modelling	Na-Cl or $Na\text{-}Cl\text{-}SO_4$, increasing Cl with depth, to 0.33 M, Recent or Pleistocene water isotopes, except deep, high Cl, possible Mesozoic marine.

17.3 Scaling issues

The spatial variation of matrix pore-water chemistry throughout a formation can be defined by judiciously spaced point samples from subsurface boreholes or core because the slow rate of matrix flow allows time for water-rock equilibrium to occur so water chemical changes are gradual.

Fracture water chemistry may change more rapidly with space and time because of the higher flow rates and water-mass mixing due to natural flow or disturbances during borehole testing and sampling. It may also be difficult to assess how well fracture water chemistry represents that of matrix pore-water. The extent to which samples of fracture water are representative of water from the entire region of host rock relevant to PA must be carefully evaluated.

17.4 Scientific level of understanding

Areas that require understanding include:

- techniques to characterise formation water,
- understanding of the water-rock reactions that are the local controls on the water chemistry,
- flow system and palaeohydrologic controls on water chemistry; and
- interaction between fracture and matrix water chemistry.

Characterisation of water chemistry begins with samples collected as described above. The sample quality decreases from borehole samples through squeezing and is least for inferences from the rock properties. In any case, such easily disturbed properties as pH, redox potential and dissolved gas concentrations will generally have to be inferred from modelling, except possibly for borehole samples. With careful experimental design, it should be possible to collect sufficient information to characterise the water chemistry in any type of argillaceous rock.

Because of the fine grain size of argillaceous rocks and the relatively long residence time of their pore-water, the assumption that water-rock chemical equilibrium prevails seems acceptable. Modelling of the Opalinus and Boom Clays in which the pore-water chemistry is well defined certainly supports this assertion. The principal minerals and reactions are common to all argillaceous rocks, but certain properties such as the cation exchange characteristics will be specific to individual formations and to the sample locations within them.

The flow system and palaeo-hydrogeology will largely determine the concentrations of solutes such as Cl and Br that are not controlled by water-rock reactions. In the Opalinus Clay at Mont Terri, for example, the Cl origin can be established as seawater and its concentration variation across the formation can be interpreted as diffusion to adjacent units in which fresh ground waters are present. In cores from the Benken borehole, there are fluid inclusions in quartz cements in sandy layers in the Opalinus Clay with salinities of 6.5-7.5 wt% NaCl(eq), i.e. well above seawater values. The formation there seems to have experienced a highly saline phase, perhaps related to dissolution of the underlying Triassic salt beds. Also, the Cl-Br ratios are not those of seawater in the Benken borehole. In the Palfris Formation at Wellenberg, the Cl may be associated with the last metamorphic fluids affecting the region and the present decrease in Cl concentration toward the surface related to the greater fracture flow developing near the surface.

The detailed relationship between fracture and matrix pore-water has not been evaluated at any site. This is because of the difficulties of fully defining fracture flow systems themselves (these may be absent in many less indurated formations) and because rocks that are indurated enough to support the development of substantial fracturing are generally too stiff to permit ready characterisation of the matrix pore-water chemistry.

17.5 Linked FEPs

FEP 1	Advection/dispersion
FEP 7	Units over- and underlying the host formation: local and regional hydrogeologic framework
FEP 8	Diffusivity
FEP 10	Ion exclusion
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 18	Dissolution / precipitation of solid phases
FEP 20	Ion exchange
FEP 21	Surface complexation
FEP 22	Thermodynamic and kinetic modelling data
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 26	Oxidation of the host rock
FEP 28	Effects of repository components on pore-water chemistry in the host rock

FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 31	Thermal effects on mineral stability and pore-water composition
FEP 43	Off-diagonal Onsager processes except chemical osmosis
FEP 44	Chemical osmosis
FEP 45	Gas dissolution and chemical interactions between gas and pore-water
FEP 49	Microbiological perturbations
FEP 50	Past burial history

17.6 Understanding from a PA perspective and treatment in PA

Generally, water chemistry is not explicitly included in PA analyses. However, it provides information important for site characterisation and therefore supports the design of the system for which the PA modelling is being performed. With the possible exception of the relationship between fracture and pore-water chemistry, this FEP is sufficiently well understood for this purpose.

Formation water chemistry is also important in choosing the values of certain transport parameters used in PA. These include diffusion properties, especially the porosity, and the solubilities and sorption properties of radionuclides. Water similar to pore-water is often used as the matrix in which laboratory determinations of site-specific formation properties are carried out. Certain formations, e.g. the Opalinus Clay at Mont Terri and the Boom Clay at Mol, have been sufficiently well characterised that salinity, pH and redox properties required to establish the transport properties are available. This is less true of formations and sites that had received only superficial study, and fractured systems like those at the Palfris Formation at Wellenberg and the Toarcian-Domerian at Tournemire.

17.7 Available reviews

The principles and practice of pore-water characterisation in argillaceous formations are reviewed by Sacchi & Michelot (2000). The extensive investigations at Mont Terri are described and compared, and the strengths and weaknesses of the various techniques used are evaluated by Pearson *et al.* (2003). The use of pore-water chemistry in choosing transport and other parameters for PA applications is addressed in several reports cited in the discussions (FEPs 18-21). Site- and formation-specific reviews and summary reports are given above.

17.8 Planned work

Formation/site	Planned activities
Callovo-Oxfordian at Bure	Extensive programme during and after the construction of the underground research laboratory
Opalinus Clay at Mont Terri	Circulate artificial pore-water in subsurface borehole and monitor changes from reactions with formation
Boom Clay at Mol	Improvement of subsurface instrumentation to minimise redox artefacts; squeezing of additional core

17.9 Overall evaluation

Pore-water chemistry is an important FEP in support of both PA and site characterisation. It is needed to adapt laboratory-measured sorption parameters to field conditions for use in PA. The spatial distribution of pore-water chemistry is a result of the hydrogeologic history of the region and is evidence of site stability.

18. DISSOLUTION/PRECIPITATION OF SOLID PHASES (FEP A2.2.5)

18.1 Definition and generalities

This FEP refers to the process by which solids dissolve in and/or are precipitated from solutions. Dissolution/precipitation reactions occurring during diagenesis and metamorphism can change the fabric of porous media and fractures, and minerals found in the formation may reflect diagenetic and metamorphic events. The occurrence and extent of these reactions may affect and be affected by the pH and redox potential of the water-rock system. This is likely to be particularly important in the excavation-disturbed zone (EDZ) where oxidation is probable (FEP 26).

Dissolution/precipitation in the context of this FEP refers to pure phases. Solid solution and co-precipitation are discussed in FEP 19. These processes are relevant to the far field in connection with site characterisation and nuclide transport properties for PA, as well as for the affected field in connection with the excavation-disturbed zone (EDZ).

18.2 Site-specific experimental information

Mineralogical descriptions of matrix rock and fracture fillings (FEP 14) and knowledge of the controls on fracture and matrix water chemistry (FEP 17) provide information about the precipitation/dissolution of minerals *in situ*. Additional reactions may occur when the host rock is exposed to the atmosphere during the construction of the underground research laboratory or disposal facility, in the EDZ (FEP 26), or in core samples, for example.

Solids that could limit radioelement concentrations are not generally observed in site studies. Instead, the possibility of their formation is inferred from the geochemistry of the water-rock-waste system and geochemical thermodynamic modelling (FEP 22).

Reported examples of dissolution/precipitation include:

Formation/ site	**In situ precipitation/dissolution**	**Reference**
Toarcian-Domerian at Tournemire	Calcite infills occur in fractures and faults.	(Boisson *et al.*, 1998, Mathieu, 1999, Mathieu *et al.*, 2000)
Opalinus Clay at Mont Terri	Carbonate re-crystallisation during diagenesis affecting pore-water Mg/Ca, Ca/Sr ratios. Rarely: precipitation of fracture-filling calcite ± celestite.	Pearson *et al.*, (2003)
Opalinus Clay in the Zürcher Weinland	Diagenetic cements are rare and occur only in sandy laminae. The bulk of the formation does not have cements. Fracture minerals are rare and volumetrically insignificant. The include mainly calcite and traces of barite, quartz and celestite.	Nagra (2002)
Mizunami Group at Tono	Carbonate mineral reactions to depth of 60 m.	Shikazono & Utada (1997)
Palfris Formation at Wellenberg	Four generations of fracture-filling calcite (± quartz) represent stages of deformation and water-rock interaction during Alpine metamorphism. Calcite in fractures is very abundant and accounts for several vol% of the whole formation.	Nagra (1997), Mazurek (1999)

Calcite is by far the most abundant fracture-filling mineral. There is a direct correlation between the degree of induration and the abundance of fracture infills. In weakly and moderately indurated formations (Boom Clay, Opalinus Clay, Toarcian-Domerian at Tournemire, Callovo-Oxfordian at Bure), they are volumetrically quite insignificant (less than 1 permil of the rock volume). In strongly indurated formations (e.g. Boda Clay Formation at Mecsek, Palfris Formation at Wellenberg), they become more abundant and may account for several percent of the rock volume.

18.3 Scaling issues

The observations cited in Section II, Chapter 18.2 are made at the hand-specimen or microscopic scale, but cover the full observable extent of the formations. The conclusions are applicable for PA analyses at all scales, from the short distances needed for considering the excavation-disturbed zone to the long distances required for far-field transport modelling.

18.4 Scientific level of understanding

The chemistry of dissolution/precipitation reactions of relatively simple pure phases such as carbonate and sulphate minerals is well understood and such reactions can be modelled with confidence if appropriate thermodynamic data are available (FEP 22). Reactions affecting the EDZ will be driven by oxidation processes (FEP 26). Redox modelling may be less definitive because of uncertainties in thermodynamic data and the need to consider reaction kinetics in some cases. Changes in clay-mineral assemblages in response to changing formation chemical and physical environments are known semi-quantitatively.

Solubilities of elements of concern in PA may be controlled by the precipitation of solids. The properties and even the identities of possible controlling phases for many elements (e.g. the actinides) are not well known so that solubilities used in PA (or the thermodynamic data from which such solubilities are calculated) must be estimated (Hummel & Berner, *in press*) (FEP 22).

18.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture water composition
FEP 22	Thermodynamic and kinetic modelling data
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 26	Oxidation of the host rock
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 31	Thermal effects on mineral stability and pore-water composition
FEP 49	Microbiological perturbations
FEP 50	Past burial history
FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)

18.6 Understanding from a PA perspective and treatment in PA

The process of dissolution/precipitation is not modelled specifically in PA analyses of the far field. However, concentration limits for radionuclides are used in the affected field of some PA models, These are based on solubilities calculated from formation water chemistry and other site characteristics. Even if solubility limits are not explicitly included in a PA model, solubilities are considered in evaluating retardation (sorption) parameters used in virtually all PA models.

Immobilisation of safety-relevant nuclides by precipitation of solid phases is generally considered a potential retardation mechanism (NEA, 2002a). However, such a process generally occurs in response to geochemical gradients (e.g. redox state, water composition). In argillaceous rocks, (except at boundaries with the EDZ or adjacent formations) the geochemical conditions in the far field are buffered by solids (FEP 17), and thus sharp gradients, such as those occurring at redox fronts, are unlikely.

18.7 Available reviews

None reported.

18.8 Planned work

Formal mineralogical characterisation of the precipitation/dissolution history will by a part of each site and formation study. Successful geochemical reaction modelling of precipitation/dissolution requires reliable thermodynamic data. Because data for many solids of PA relevance (e.g. those of the actinides) are marginal at best, thermodynamic data base development is a continuing process (see FEP 22).

18.9 Overall evaluation

From a generic point of view, the process of dissolution/precipitation is important as a control on the solubility of certain elements included in PA analyses. From a site-specific point of view, examination of existing minerals can illuminate the geologic history of the formation and site area and guide the regional description of the site used in PA. Dissolution/precipitation as a result of repository excavation, construction and operation can affect the transport properties of the repository and adjacent host rock.

19. SOLID SOLUTIONS/CO-PRECIPITATION (FEP A2.2.6)

19.1 FEP definition

Co-precipitation is a process by which two or more chemical components are simultaneously and permanently incorporated into a single solid during its precipitation from solution, either in amorphous or crystalline compounds (Curti, 1997). The term solid solution refers to a special type of co-precipitation in which a foreign component substitutes in regular lattice sites of crystalline compounds. This definition excludes processes of surface complexation and ion exchange by which an ion can be released into solution without dissolution of the solid or replacement by another ion(s) of like charge.

The best-known, naturally-occurring solid solutions include carbonate minerals (e.g. substitution of Fe^{+2} for Mg^{+2} in dolomite forming ankerite, and the trace concentrations of alkaline earth elements, Fe^{+2}, Mn^{+2} and other ions of similar size and charge in the calcite or aragonite lattice). Clay mineral groups are sometimes treated as solid solutions, but the mechanisms of their precipitation and dissolution are too poorly understood to consider them in PA. Elements of PA interest can be immobilised or retarded by co-precipitation in solids such as ferrihydrite that may form during degradation of repository materials, and other solids that may form during interactions between pore-waters and repository fluids, especially those of high pH that can issue from cement.

This FEP should be considered relevant for all far-field features containing carbonate and clay minerals. These include not only the matrix of argillaceous rocks but also surface coatings and infill of water-conducting fractures, which are commonly enriched in carbonate and clay minerals.

Co-precipitation in the affected field if cement is present should be considered relevant regardless of the type of host rock involved.

19.2 Site-specific experimental information

There appears to be no site-specific information on co-precipitation with clay minerals or in the affected field from *in situ* experiments. However, there are indications from natural analogue and laboratory studies, particularly of carbonate minerals, that this process is likely to be important to PA (Curti, 1997).

Type of Study	Finding	Reference
Natural analogue: Poços de Caldas, Brasil	Co-precipitation of U, Zn and REE elements in ferrihydrite was identified. Sr concentrations in ground water are controlled by fluorite dissolution (*i.e.* co-dissolution of Sr).	Bruno *et al.* (1996)
Natural analogue: Maqarin, Jordan	Trace element distribution in ground water cannot be reconciled with solubilities of pure phases.	Smellie (1998)
Natural analogue: Palmottu U deposit in crystalline rock, Finland	Fracture-filling calcite contains substantial amounts of U.	Read *et al.* (2001a)
Clay minerals formed at low temperatures: Fe-rich sediments; Lateritic soils	Strong partitioning of divalent metals, especially Ni, into solid phase in natural minerals and laboratory syntheses.	Trescases (1997), Curti (1997), Savage (1994), Besset (1978), Borchert (1965), Halbach (1969), Velde (1989), James (1966), Grauer (1990), Decarreaux (1985), Harder (1978, 1989)
Various sources of data	Co-precipitation of PA-relevant elements was compiled on the basis of field and laboratory data: Ra, Sr incorporated into calcite Se incorporated into pyrite Ni incorporated into pyrite, Fe/Mn hydroxides, calcite.	Heath (2002), Smellie (2002), Stipp (2002)

A thermodynamic modelling approach based on the minimisation of Gibbs free energy (GEM) has been developed and considers equilibria of dissolution/precipitation reactions, co-precipitation and sorption (Karpov *et al.*, 2001, Kulik, 2002). The use of the chemical potentials of independent components allows solving the problem of determination of the Gibbs free energy of formation of compounds from their known contents in the systems, and *vice versa*. For example, the method has been applied to marine authigenic carbonate – seawater equilibria. Based on the known concentrations of Mn, Ca, Fe, Mg, Sr, Ba, C and O in carbonate and co-existing seawater, solid activity coefficients of the end-members in the non-ideal solid solution (Mn, Ca, Mg, Sr, Ba, Fe)CO_3 could be estimated, and Margules interaction parameters were derived (Kulik *et al.*, 2000). The method can be potentially expanded to the study of other natural analogues to constrain the partitioning of radionuclides between the solid and liquid phases.

19.3 Scaling issues

None reported.

19.4 Scientific level of understanding

Although solid solution/co-precipitation is widely recognised to be an important mechanism for radionuclide retention (see e.g. Nagra, 1995, p. 172), the current level of understanding is in general low (NEA, 2002a, ch. 3.5.3). This is particularly true for clay minerals, which have a complex multiple site structure and are frequently inhomogeneous at the scale of tens of nm. For this reason, safety analyses are carried out ignoring the effects of this process. To increase the knowledge in this field to a level which would justify incorporation in PA would require a large effort in terms of both experimental and modelling work by the whole scientific community. Presently, work is being performed by different groups in order to increase the understanding of this process in terms of basic mechanisms.

Formation of solid solutions (beyond the trace element level) could also lead to modifications of key properties of clay minerals (e.g. sorption and swelling properties). These effects are presently not quantifiable due to the currently poor knowledge of the chemical changes in the clay minerals, which ultimately depend on the evolution of the repository system (e.g. groundwater composition).

The current level of understanding in the context of the retention of radionuclides in the affected field is also poor (Curti, 1997). Co-precipitation of radionuclides with CSH phases is the result of the interaction of hyperalkaline fluids with the host rock. The process is operative if a source of hyperalkaline pore-water exists. CSH phase formation and the formation of other possible secondary phases in the pH plume is understood qualitatively but not quantitatively (e.g. Smellie, 1998).

It is because of the lack of understanding of the mechanism of formation that solid solution / co-precipitation are not considered a robust retention mechanism in NEA (2002a). However, as the natural analogue results show, solid solutions once formed, as by the passage of a front emanating from a repository, appear persistent.

19.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture water composition
FEP 22	Thermodynamic and kinetic modelling data
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 26	Oxidation of the host rock
FEP 29	Interactions of hyperalkaline fluids and host rock

FEP 49 Microbiological perturbations

FEP 50 Past burial history

FEP 52 Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)

19.6 Level of understanding from a PA perspective and treatment in PA

For the reasons mentioned above, co-precipitation processes are not included in the safety assessment models. There are, however, two approaches by which radionuclide co-precipitation could be included in evaluating the solubility and/or sorption coefficients to be used for PA. If a sufficient level of knowledge is available: (1) empirical partition coefficients could be applied based on measurements of the distribution of the various radionuclides between solid and aqueous phases; (2) thermodynamic solid solution models could be used. The first method implies a very large experimental data base for the relevant nuclides and solids. There would be no need for implementation in a geochemical code but the requirement for data covering all relevant radionuclides and conditions is prohibitive. Thus, this approach would be applicable to a few critical radionuclides. The second approach is based on general thermodynamic principles and could be realised with less experimental effort. The advantage would be a broader applicability, but implementation in advanced thermodynamic codes would be required as well as the development of the additional thermodynamic modelling parameters requires (see FEP 22). In both cases, this FEP would be introduced in the safety assessment model in the form of reduced solubility limits.

19.7 Available reviews

Curti (1997) reviewed the basic concepts and initial applications of co-precipitation to radioactive waste management. The mechanisms of waste stabilisation in cementitious media are described in the review by Cocke & Mollah (1993). According to these authors CSH phases are prime candidates for heavy metal binding because of their abundance and appropriate structures.

Solid solution algorithms are included in most modern geochemical modelling programmes. Those in PHREEQC (Parkhurst & Appelo, 1999) for example, embody the theory described by Glynn & Reardon (1990) and Glynn & Parkhurst (1992).

The 2001 GEOTRAP workshop (NEA, 2002a) dealt with retention processes, including immobilisation by precipitation and co-precipitation. This topic was also taken up by one of the working groups of the workshop.

19.8 Planned work

In the context of an ongoing European project (ACTAF), an attempt will be made to systematise experimental data on the uptake of radionuclides by calcium carbonate (calcite) in terms of thermodynamic solid solution models. Although this work is not directly related to argillaceous systems, it will have a "model character" for understanding the mechanisms and main parameters controlling solid solution formation with trace elements. Calcite has been selected due to the inherent simplicity of its structure (only 1 cationic site) and its reactivity. Institutions involved: Forschungszentrum Rossendorf, University of Copenhagen, Paul Scherrer Institute. The project is scheduled to be completed by the end of 2003.

Although of less relevance to the far field, work on the co-precipitation of Sr, Ni, Eu and Th by CSH phases is in progress at the Paul Scherrer Institute. This work will be carried out until 2003, partially within the context of an ongoing European project (Ecoclay II).

19.9 Overall evaluation

Co-precipitation processes in the affected field when cement is present are likely to have a beneficial effect on radionuclide retention. However, the present status of knowledge is not sufficient to justify inclusion in PA models.

Argillaceous rocks commonly contain carbonate minerals, both in the matrix and as fracture fillings. Thermodynamic data are available for carbonate solid solutions and could be used to evaluate the affects of this process on the solubility values used in PA.

20. ION EXCHANGE (FEP A2.2.7)

20.1 Definition and generalities

Ion exchange is one of the processes underlying sorption, the other being surface complexation (FEP 21). It differs from surface complexation in that the charged sites on which it occurs represent charge imbalances in the solid lattice and do not change with external conditions. Prominent ion exchange media include zeolites, the permanent charge sites of clay minerals (predominantly on their layer surfaces), and certain artificial organic resins. Ion exchange equilibria are described by mass action equations that do not include consideration of variably-charged surfaces nor of electrostatic effects.

Ion exchange among major cations is an important control on the chemistry of water in argillaceous formations. The effects of cation exchange can also be observed in regional water chemistry changes in formations with clay-mineral contents of only a few percent.

The sorption of solutes present in trace amounts in argillaceous formations can also be described by an ion exchange model. Ion exchange is relevant to the far field in connection with site characterisation and nuclide transport properties for PA as well as to the affected field.

20.2 Site-specific experimental information

Ion exchange data on the following formations have been determined principally to permit modelling of pore-water chemistry:

Formation/site	Elements	Reference
Callovo-Oxfordian at Bure	Na, K, Mg, Ca	Andra (1999a)
Toarcian-Domerian at Tournemire	Na, K, Mg, Ca, Sr	Boisson *et al.* (1998), Cabrera *et al.* (2001)
Spanish Reference Clay in a Tertiary basin	Na, K, Mg, Ca, Sr	Ciemat (1999)
Opalinus Clay at Mont Terri	Na, K, Mg, Ca, Sr	Pearson *et al.* (2003)
Opalinus Clay in the Zürcher Weinland	Na, K, Mg, Ca, Sr	Nagra (2002)
Boom Clay at Mol	Na, K, Mg, Ca	Baeyens *et al.* (1985), Griffault *et al.* (1996)
Palfris Formation at Wellenberg	Na, K, Mg, Ca	Baeyens & Bradbury (1994)

Ion exchange data for a number of elements on pure minerals important in argillaceous formations are available in the literature (e.g. Bruggenwert & Kamphorst, 1982).

20.3 Scaling issues

Ion exchange properties are measured on point samples from core. Cation exchange is a chemical process and is not scale dependent. However, total exchange capacities will vary with the mineralogical composition of the formation and the proportions of exchangeable ions will vary with changing pore-water composition. Upscaling is feasible if the large-scale distribution of mineralogy and pore-water composition is known.

Total exchange capacity and mineral-surface area of matrix rock accessible to water in fractures depend on the accessibility of the matrix to pore-water. Water-rock interaction and ion exchange measurements are carried out on crushed samples. In principle, crushing could create or expose grain surfaces not active in the *in situ* rock so that laboratory-measured properties may not represent those of the bulk rock. Surface coatings of rocks and minerals in the field are likely to play an important role in determining the geochemical or sorption properties of formations (see for example Chapter 4 in Yariv and Cross, 1979). Because such coatings have sizes similar to the laboratory crushed rock samples, properties determined on the latter may be reasonably representative of those of the bulk formation.

Fault gouges with grain sizes similar to those of artificially crushed samples may be present as infill material in faults. Thus, laboratory-measured properties of crushed samples are likely to be representative of such materials. Such fault gouges occur in fractured formations such as the Palfris Formation at Wellenberg.

20.4 Scientific level of understanding

The importance of ion exchange as a control on the chemistry of natural waters has long been known (e.g. Way, 1852, Foster, 1950), as has the likelihood that it will retard the transport of radionuclides (e.g. Robinson, 1962). Ion exchange has been extensively studied, albeit with emphasis on the behaviour of soils rather than of consolidated rock (Sposito, 1981, 1994) and is well understood in pure systems (mainly bi-ionic clay systems). There is a vast amount of selectivity coefficient data in the open literature (e.g. Bruggenwert and Kamphorst, 1982).

The application of ion exchange models to interpret sorption measurements and extend them for use in PA is discussed by Altmann & Bruno (2001). Poinssot *et al.* (1999) and Bradbury & Baeyens (2000) quantitatively describe the concentration dependent sorption of Cs on argillaceous rock and pure clay minerals using a cation exchange model.

For a robust interpretation of sorption, the identity of the sorbing aqueous species must be known. The aqueous speciation of some elements (e.g. the actinides) is not well enough understood that the sorbing species can always be unequivocally identified. This leads to uncertainty in the extension of laboratory measurements to field conditions (Hummel & Berner, *in press*; see FEP 22).

The role of cation exchange in determining pore-water chemistry has been described for a number of argillaceous formations including the Boom Clay (Griffault *et al.*, 1996), the Palfris Formation (Baeyens & Bradbury, 1994, Pearson & Scholtis, 1994, Pearson *et al.*, 1998), the Opalinus

Clay (Bradbury & Baeyens, 1998a, Thury & Bossart, 1999 Pearson *et al.*, 2003) and in the Mizunami Group in the Tono area (Iwatsuki *et al.*, 1995).

Cation exchange algorithms are included in computer programmes used for modelling water-rock geochemical reactions and the behaviour of dissolved contaminants (see FEP 22).

Changes in water chemistry that are consistent with cation exchange, such as the tendency for the dominant cation to shift from Ca to Na and for the Na/K ratio to change with flow, can also be attributed to equilibria among different clay minerals, or to reactions with other silicate minerals such as feldspars. This approach is summarised and reviewed by Langmuir (1997, Ch. 9). Pearson & Scholtis (1995) describe the cation exchange processes that lead to the changes in water chemistry with depth in the Palfris Formation at Wellenberg. Beaucaire *et al.* (2000) model the chemistry of ground water near Mol using feldspar equilibria to control the Na/K ratio. Because of the uncertainty in data available for thermodynamic properties of clay minerals and for the kinetics of reactions among silicates, the cation exchange formalism is more widely used (see FEPs 19 and 22)

20.5 Linked FEPs

FEP 12	Colloid formation, transport and filtration
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 16	Mineral-surface area
FEP 17	Pore- and fracture water composition
FEP 22	Thermodynamic and kinetic modelling data
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 31	Thermal effects on mineral stability and pore-water composition
FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)

20.6 Level of understanding from a PA perspective and treatment in PA

Ion exchange is one of the mechanisms generally lumped under the rubric of “sorption”, the other being surface complexation (FEP 21). Generally, PA treats sorption by means of a single solid-liquid distribution coefficient (K_d approach). In many cases mechanistic understanding e.g. ion exchange, enables sorption values to be selected (calculated) for specific chemical conditions in the *in situ* host rock. A mechanistic understanding of the sorption process is used to justify and defend the selected sorption values in the sorption data bases which are used in the PA (Altmann & Bruno, 2001).

20.7 Available reviews

Altmann and Bruno (2001): Review use of thermodynamic sorption models for guiding radioelement distribution coefficient (K_d) investigations for performance assessment.

Helfferich (1962): Ion exchange. Standard textbook.

Bolt (1982): Description of physico-chemical ion exchange models (Chaps. 2-6).

Sposito (1981, 1994): Chemical equilibria and kinetics in soils.

References to the treatment on ion exchange (and other sorption processes) in geochemical modelling programmes are given in FEP 22.

20.8 Planned work

Work planned by Nagra/PSI includes pore-water chemistry and sorption investigations on crushed Opalinus Clay from the Benken borehole (laboratory experiments), and modelling the pore-water chemistry and sorption results on Opalinus Clay.

20.9 Overall evaluation

A description of radionuclide uptake processes using a formalism such as ion exchange provides support and justification for the sorption data bases used in PA. In systems for which direct experimental data are available for appropriate mineralogical and geochemical conditions, experimental data may be used directly for PA. For systems in which mineralogy or geochemical conditions may change with space or time or which are not accessible in the laboratory, it will be important to develop (quasi) mechanistic understanding such as ion exchange on clay minerals. Such understanding will permit extrapolations of sorption data bases to other mineralogical and chemical conditions.

Inclusion of the ion exchange process and availability of site-specific ion exchange data are necessary for the geochemical modelling needed to characterise pore-water in argillaceous media.

21. SURFACE COMPLEXATION (FEP A2.2.8)

21.1 Definition and generalities

Surface complexation is one of the processes underlying sorption, the other being ion exchange (FEP 20). Surface complexation is the reversible binding of dissolved species on surfaces with charges that vary with solution chemistry and crystal-chemical effects. Both chemical complexation (co-ordination) and electrostatic interaction with surfaces occur. Prominent substrates for surface complexation include metal oxides and hydroxides of Fe (ferrihydrite, goethite), Al (α, δ alumina) and Si (amorphous silica, quartz), broken bond sites on clay-mineral edges, and organic substances such as humic and fulvic acids and polysaccharides.

Surface complexation models are widely applied in studying the movement of pollutants in surface waters and shallow ground waters. Surface complexation occurs in all types of argillaceous media and is relevant in the far field for site characterisation and nuclide transport properties for PA. The processes involved are well understood and can be adequately modelled for the non-clay mineral phases that provide the main sites for surface complexation, such as hydrous ferric oxide minerals (Dzombak & Morel, 1990), manganese oxides and some silicates. However, surface complexation processes are less well understood on clay minerals and in complex media containing carbonates or organics (Davis & Kent, 1990, Stumm, 1992). Ion (cation) exchange i.e. electrostatic attraction onto constant-charge surfaces may be a more important process than surface complexation for univalent, divalent and some trivalent cations for the basal planes of clay minerals.

21.2 Site-specific experimental information

Laboratory sorption measurements have been made for elements of importance for nuclear waste disposal on samples of formations under study as potential host rocks. Many of these have not been interpreted in terms of the underlying processes, i.e. they are only applicable to the rocks from which the data were derived, while extrapolations to other rock formations are difficult.

Sorption measurements interpreted in terms of surface complexation models or of two-site surface complexation and ion exchange models are available for a number of pure solids, minerals and bulk clay rocks. These represent the primary sources of sorptive capacity of argillaceous rocks. They can be used with the mineralogical composition of target host rocks to generate site-specific sorption data (Bradbury & Baeyens, 1997).

Mineral or solid	Elements	Reference	Comments
Hydrous ferric oxide	Ag, Ba, Ca, Cd, Co, Cr(III), Cu, Hg, Ni, Pb, Sr, Zn, As(V), As(VII), BO_3,CrO_4, PO_4, SeO_3, SO_4, S_2O_3, VO_4	Dzombak & Morel (1990)	Standard reference on surface complexation modelling
Illite, calcite	Cs, K, Sr, Ra, Ni, Co, Pd, Ag, Pb, Sn, Mo, Nb, Tc, Po, Am, Ac, Cu, Th, U, Np, Pu, Pr, I, Cl, C(org), C(inorg)	Bradbury & Baeyens (1997)	Review of literature data supporting selection of K_d values for Palfris Formation at Wellenberg
Numerous	Numerous	Altmann & Bruno (2001)	Summary of presentations at 1997 Oxford meeting

21.3 Scaling issues

Surface complexation is a chemical process and so is not scale dependent. However, surface complexation capacities will vary with the mineralogical composition of the formation and the proportions of complexed ions will vary with changing pore-water composition. Upscaling is feasible if the large-scale distribution of mineralogy and pore-water composition is known.

Water-rock interaction and sorption measurements are carried out on crushed samples. In principle, crushing could create or expose grain surfaces not active in the *in situ* rock so that laboratory-measured properties may not represent those of the bulk rock. Surface coatings of rocks and minerals in the field are likely to play an important role in determining the geochemical or sorption properties of formations (see for example Chapter 4 in Yariv and Cross, 1979). Because such coatings have sizes similar to the laboratory crushed rock samples, properties determined on the latter may be reasonably representative of those of the bulk formation.

Fault gouges with grain sizes similar to those of artificially crushed samples may be present as infill material in faults. Thus, laboratory-measured properties of crushed samples are likely to be representative of such materials. Such fault gouges occur in fractured formations such as the Palfris Formation at Wellenberg.

21.4 Scientific level of understanding

Surface complexation as a sorption process has been extensively studied and is rather well understood on pure minerals (mainly oxide systems, e.g. Schindler & Stumm, 1987, Dzombak & Morel, 1990). There are multitudes of surface complexation models in the open literature and generally accepted methodology for describing sorption by surface complexation in natural systems. Comprehensive reviews of methods of chemical modelling for ion sorption in natural systems are given by Davis & Kent (1990) and Goldberg (1992). However, there exists no uniform treatment of surface complexation.

The surface complexation behaviour of clay minerals, with several types of sorption sites, is less well understood. Sorption measurements can often be equally well interpreted using models based on contradictory physical theory (e.g. comments of Morel & Kraepiel, 1997 on Baeyens & Bradbury, 1997).

In unfractured argillaceous formations, the dominant transport mechanism is likely to be diffusion. The physical and mathematical models used to describe diffusional transport must be consistent with the models used to interpret sorption data. The problems of deriving sorption parameters from laboratory K_d measurements that are consistent with those from diffusion measurements have been explored for compressed bentonite considered as repository backfill, but have not yet been resolved. There are strong analogies between the properties of compressed bentonite and natural argillaceous media that should be considered when seeking understanding of the behaviour of either.

Surface complexation on organic matter could be an important retardation mechanism in formations such as the Boom Clay with significant organic carbon contents. However, too little is known about the process for it to be included in PA.

Due to the limitations of spectroscopic techniques, the existence of surface complexation on clay-mineral/natural organic surfaces is yet to be confirmed – here, surface complexation is more a model concept than a real process. The method of calculating sorption as the sum of different processes, i.e., ion exchange, surface complexation, surface precipitation, is model dependent.

21.5 Linked FEPs

FEP 12	Colloid formation, transport and filtration
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 15	Natural organics, complexation: *Increasing degree of complexation of radionuclides by humic substances may lead to decreasing sorption. Neglecting the effect of radionuclide complexation by humic substances may lead to an over-estimation of sorption (over-optimistic).*
FEP 16	Mineral-surface area
FEP 17	Pore- and fracture water composition
FEP 22	Thermodynamic and kinetic modelling data
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 26	Oxidation of the host rock
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 30	Organics from waste and their effect on transport properties of the host rock
FEP 31	Thermal effects on mineral stability and pore-water composition
FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)

21.6 Level of understanding from a PA perspective and treatment in PA

PA models do not include surface complexation directly but treat sorption by means of a single solid-liquid distribution coefficient (K_d approach). This approach is generally regarded as sufficient for PA purposes. Uncertainties are covered by the choice of conservative (i.e. low) K_d

values. In many cases mechanistic understanding based on surface complexation and ion exchange is used to justify and defend the values selected for the sorption data bases used in PA (Altmann & Bruno 2001, Bradbury & Baeyens, 1997).

In the Spanish preliminary PA in clay (Enresa, 1999) the input data used to model the transport through the clay formation are the apparent and effective diffusion coefficients (D_e and D_a). For modelling, these data are transformed into values of the pore diffusion coefficients (D_p), accessible porosity and distribution coefficients (K_d) that reproduce the desired values of D_e and D_a. In this assessment, the radionuclides that cause the greatest doses are two non-sorbing species: ^{129}I and ^{36}Cl.

21.7 Available reviews

There are numerous reviews in the open literature on surface complexation and on sorption. The review of the use of thermodynamic sorption models for guiding radioelement distribution coefficient (K_d) investigations for PA by Altmann and Bruno (2001) is particularly timely and relevant. Reviews specifically on surface complexation modelling include the definitive 1990 reports by Dzombak & Morel (1990) and Davis & Kent (1990). More recent short reviews developing the surface complexation modelling approach is included in Davis *et al.* (1998). These authors discuss the application of the surface complexation concept to rock surfaces with several minerals providing surface complexation sites and review the success of non-electrostatic sorption models. Sposito (1981, 1994) describes surface complexation among other chemical processes active in soils. References to the treatment of surface complexation and ion exchange in geochemical modelling programmes are given in FEP 22.

21.8 Planned work

Work is planned in Switzerland to continue laboratory investigations of crushed Opalinus Clay samples from the Benken borehole and to perform surface complexation modelling of the sorption results on Opalinus Clay from Mont Terri and the Benken borehole.

In the ongoing TRANCOM-Clay phase II project, a 3-year study of interaction between radionuclides and Boom Clay is planned for batch, column, and *in situ* experiments. The objective is to study the effect of natural organic matter on the mobility of radionuclides under a reducing condition. The proposed project involves SCK•CEN (co-ordinator) and K.U.Leuven (B), University of Loughborough (UK), Galson Sciences (UK) and Ecole des Mines (Armines, F).

21.9 Overall evaluation

Sorption, quantified as K_d values, is extremely important in describing radionuclide transport behaviour in PA models. K_d values are commonly based on laboratory batch experiments with pure phases or on bulk host rock, or found from D_a and D_e values measured on host rock samples. PA models use K_d models directly. In the case that *in situ* conditions cannot be satisfactorily simulated in the laboratory or if more than empirical support is desired for data used for PA, (quasi) mechanistic explanations such as surface complexation for radionuclide uptake processes on (hydr)oxides and clay minerals are useful. Such understanding makes it possible to justify and defend values selected for the sorption data bases used in PA. Further, the influence of changing mineralogies and water chemistries can be predicted over a large range.

22. THERMODYNAMIC AND KINETIC MODELLING DATA (FEP A2.2.9)

22.1 Definition and generalities

Thermodynamic data are used to support equilibrium modelling of geochemical reactions that occur throughout the waste isolation system. They include temperature-dependent values of equilibrium constants for the dissolution of solids and gases in water, for redox reactions, and for the formation of solute complexes (ion pairs) in solution. Species-specific values for parameters of the activity coefficient expressions chosen for the modelling of the solution and of solids must also be known. Data for ion exchange and surface complexation equilibria are considered in FEPs 20 and 21.

Most geochemical programmes model equilibrium for water-mineral reactions controlling the matrix water chemistry of argillaceous formations. This is acceptable because of the fine grain size of the minerals and the long residence times of pore-water in such poorly transmissive media. Geochemical equilibrium models are not used directly in assessing site performance, but are required for site characterisation activities (FEP 17) and for developing parameter values used in PA (FEPs 18-21). The results of geochemical modelling are no more reliable than the thermodynamic data supporting them.

Kinetic data include temperature-dependent reaction rates. The assumption of geochemical equilibrium may not be justified for reactions among silicate minerals in the host rock and for these reactions kinetic data may be required.

Sorption K_d values actually used in PA are not included in geochemical equilibrium models and so are not considered to be thermodynamic data as the term is used in this FEP. However, both ion exchange and surface complexation processes are included in most current geochemical modelling computer programmes.

22.2 Site-specific experimental information

In principle, thermodynamic data are generic and should be valid for use at all sites. A number of data compilations have been made, which are so widely known they do not require citations here. There are also critically reviewed compilations of data of particular relevance to nuclear programmes, such as the NEA reviews for uranium (Grenthe *et al.*, 1992), americium (Silva *et al.*, 1995), plutonium and neptunium (Lemire *et al.*, 2001) and for Ni, Se and organic ligands (in progress). Many nuclear waste programmes, including Nagra (Hummel *et al.*, 2002a,b), JNC and Nirex (Cross & Ewart, 1990) have generated thermodynamic data sets for their specific use.

Geochemical modelling programmes such as EQ3/EQ6 (Wolery, 1992), MINEQL (MINSORB) (Westall *et al.*, 1976; Bradbury & Baeyens, 1994), MINTEQA2 (Allison *et al.*, 1991; USEPA 1999a, b), PHREEQC (Parkhurst & Appelo 1999), CHEMAPP (Eriksson *et al.* 1995, 1997) and The Geochemist's Workbench® (Bethke, 1994) make use of these data and include data bases of their own. Bethke (1996, App. 1) and Langmuir (1997) provide more comprehensive lists of geochemical modelling software and give sources for further information about each programme.

22.3 Scaling issues

Because the thermodynamic data referred to in this FEP are generic, scaling is not an issue.

22.4 Scientific level of understanding

Although a great many thermodynamic data are available in the general literature and specifically for nuclear waste work, the data sets are generally not complete and include considerable uncertainties. These uncertainties are particularly evident in data for elements commonly present in trace quantities and may lead to uncertainties in solubilities, for example, that may need to explicitly considered in PA. Missing data may lead to incorrect calculation of the aqueous speciation information used to extend and justify laboratory K_d data for PA use.

To overcome the problem of missing data, problem-specific estimates of data may be needed to rationally develop solubility values and extend sorption data. The relationship between thermodynamic data bases and parameter values used in PA is described by Hummel & Berner (*in press*).

Kinetic data for mineral precipitation/dissolution are far from complete. Kinetics of redox reactions are not well understood.

22.5 Linked FEPs

In principle, thermodynamic and kinetic data are independent of all other FEPs. However, the specific needs for such data is constrained by the minerals and the geochemical and thermal environments, which in turn are defined by the following FEPs:

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture water composition
FEP 26	Oxidation of the host rock
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 31	Thermal effects on mineral stability and pore-water composition

22.6 Level of understanding from a PA perspective and treatment in PA

Thermodynamic data are not used directly in PA. However, the geochemical models they support are required to develop the knowledge of pore-water chemistry needed for site characterisation and to guide the conditions chosen for laboratory experiments, and to evaluate the solubility and sorption values actually used in the PA.

Carefully compiled thermodynamic data bases (e.g. Hummel *et al.*, 2002b) contain sufficient data of quality adequate to permit modelling of pore-water chemistry for PA purposes. On the other hand, there is insufficient and/or only poor quality thermodynamic data for many of the less common elements, particularly the actinides and other radioelements, that are important for PA calculations. Techniques for developing thermodynamic data are well understood (e.g. Hummel *et al.*, 2002b), but not fully applied at present. Thus, techniques to identify and evaluate missing data are used instead (Hummel and Berner, 2002).

22.7 Available reviews

Thermodynamic data base selection and contents development are discussed in many standard textbooks such as Stumm & Morgan (1996), Nordstrom & Munoz (1994) and Langmuir (1997). The NEA volumes and the reports describing thermodynamic data bases used in various waste management programmes listed in Section II, Chapter 22.2 also discuss the data selection process. The recent Nagra/PSI data base report includes a particularly valuable discussion of data base consistency (Hummel *et al.*, 2002a).

22.8 Planned work

Thermodynamic data bases are under continuous development in many programmes.

22.9 Overall evaluation

Thermodynamic data are required to support the geochemical modelling that is part of all waste management programmes. Such data bases accompany all widely-used geochemical modelling programmes. Data bases for waste management use may need additional constituents and will certainly need to be checked for internal consistency and precision before applying them to develop values for parameters used in PA.

23. PALAEO-HYDROGEOLOGY OF THE HOST FORMATION AND OF EMBEDDING UNITS (FEP A3.1, C1.1.1)

23.1 Definition and generalities

This FEP refers to the palaeo-hydrogeology of the site region as an attribute of system understanding. Palaeo-hydrogeology in this context refers to those processes and events that have occurred in the past and contributed to the present state of the system, particularly the evolution of the hydraulic regime under the influence of diagenesis and deformation. It is parallel to FEP 24, "Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units". This FEP is relevant to the far field in connection with site characterisation and nuclide transport properties for PA, and to the affected field in connection with boundary conditions for analysis of the engineered barrier system.

The palaeo-hydrogeologic history of a site is a synthesis of information developed for other FEPs (see below).

23.2 Site-specific experimental information

Descriptions of palaeo-hydrogeology have been synthesised for the following sites:

Formation/ site	Overview of palaeo-hydrogeology	Reference
Opalinus Clay in the Zürcher Weinland	The Mesozoic evolution is characterised by sedimentation and subsidence of the basin. With some minor exceptions, conditions are marine. Due to compaction, pore-waters are expelled (namely in argillaceous formations), which results in advection at least in the aquifers. Evaporitic brines migrate into the adjacent formations (e.g. documented by highly saline fluid inclusions in the Opalinus Clay). Low relief, most likely only small hydraulic gradients. Due to basin inversion in the Early Tertiary (65-29 Ma), Cretaceous sediments are eroded, and a karst aquifer develops in the Malm (Late Jurassic). Diffusive exchange of solutes with the underlying formations (such as the Opalinus Clay) is likely, given the large time scales involved. The Opalinus Clay looses some Cl and He at this stage. Low relief, slightly enhanced hydraulic gradients. Late Oligocene – Early Miocene (29-20.5 Ma): Subsidence and sedimentation of Molasse detritus. Complex hydrochemical conditions in the Malm aquifer (fresh - brackish, affected by evaporation).	Nagra (2002)

Formation/ site	Overview of palaeo-hydrogeology	Reference
	Early – Late Miocene (20.5-10 Ma): Continued subsidence and sedimentation, low relief, low hydraulic gradients. Generation of overpressures in argillaceous units due to compaction. Highly saline waters in Mesozoic aquifers, partial infiltration of seawater into the Malm aquifer. Late Miocene – Pliocene (10-2.6 Ma): Inversion of the basin, uplift and erosion, substantial relief, enhanced hydraulic gradients. Partial dissipation of overpressures. Beginning of infiltration of meteoric waters into deep aquifers, followed by diffusive exchange with argillaceous formations. Pleistocene – Holocene (2.6-0 Ma): Continued uplift, infiltration of meteoric waters and diffusive exchange with argillaceous units. A diffusion profile of $\delta^{18}O$, $\delta^{2}H$ and Cl developed in the Opalinus Clay in the last 0.5-2 Ma (Gimmi, 2002).	
Boom Clay at Mol	The PHYMOL project (Marivoet *et al.*, 2000) is a palaeo-hydrogeologic study of the Mol region based on hydraulic data and on isotope and chemical data, also integrating the earlier ARCHIMEDE project. Tritium is present in water overlying the Boom Clay and in the recharge areas of underlying aquifers. $^{14}C_{\text{fulvic acid}}$ indicates residence times from 0 to 30 ka in underlying aquifers, and suggests reduced recharge during the coldest period, from about 15 to 22 ka. Water isotopes and noble gas contents also indicate palaeo-climatic effects on the deeper waters. Attempts to model ^{14}C and ^{18}O values from about -130 ka to the present are hindered by only a limited number of useful observations and uncertainties in the estimates of the palaeo-conditions (temperatures and corresponding ^{18}O contents in meteoric recharge, the extent of ice sheets and permafrost, the sea-level drop, topographic changes and river erosion and above all the infiltration rate) used in the modelling. H and O isotopic data and chemistry of pore-water from the Boom Clay and underlying Rupelian aquifer indicate that the latter is a mixture of *in situ* pore-water with water of marine origin equilibrated with the formation. Other aquifer water appears not to be equilibrated with the rock. Since 1.6 Ma ago, the Campine Basin has evolved from a marine to a continental environment, and fresh water started to infiltrate into the aquifers surrounding the Boom Clay.	Griffault *et al.* (1996), Philippot *et al.* (2000), Pitsch & Beaucaire (2000), Marivoet *et al.* (*2000*), Wemaere *et al.* (2000)

23.3 Scaling issues

Palaeo-hydrogeology integrates events and processes that occurred over large scales in space (site scale to regional scale) and in time (ka – Ma). Palaeo-hydrogeological arguments can be used to support extrapolations of hydrodynamic and hydrochemical processes that were originally characterised on small spatial and temporal scales.

23.4 Scientific level of understanding

Reconstructing the palaeo-hydrogeology of a region is straightforward if the information described in Section II, Chapter 23.2 is available. The quality and reliability of the reconstruction depends directly on the amount and quality of the supporting data.

23.5 Linked FEPs

This FEP synthesises the interaction and the effects of most FEPs of the A (Undisturbed system) and C (Long-term evolution) groups.

23.6 Level of understanding from a PA perspective and treatment in PA

The site properties and attributes on which a PA is based must be consistent with its palaeo-hydrogeology. Events occurring during the hydrogeologic evolution of a site may also suggest scenarios for future site behaviour.

23.7 Available reviews

NEA (1993, 1999b).

23.8 Overall evaluation

The synthesis called for by this FEP requires evaluation of site characterisation data from a number of disciplines. Its successful completion addresses the quality, completeness and internal consistency of the supporting data and adds credibility to the site model defined for PA.

24. EVOLUTION OF PORE-FLUID (WATER AND GAS) CHEMISTRY AND MINERALOGY IN THE HOST FORMATION AND IN EMBEDDING UNITS

(FEP A3.2, C1.1.2)

24.1 Definition and generalities

This FEP addresses the evolution of fluids such as water and gases and water-rock interactions during past basin evolution. It is a synthesis of information on the present fluid chemistry and mineralogy of the formation. The latter includes the identity of minerals present in the formation, their distribution and fabric, their chemical and isotopic compositions and other attributes such as fluid inclusions that may indicate presently or previously active water-rock reactions and transport processes. Likewise, the absence of certain minerals or reactions may mark the limits of penetration of past fluids. Knowledge of past and ongoing processes of fluid and mineral evolution will guide selection of the processes that should be considered in PA.

This FEP is parallel to FEP 23, “Palaeo-hydrogeology of the host formation and of the embedding units”. It is relevant to the far field in connection with site characterisation and the nuclide transport properties for PA, and to the affected field in connection with the boundary conditions for analysis of the engineered barrier system.

Fluids affecting the formation during its geological history include waters of deposition, diagenetic, metamorphic and magmatic fluids, and infiltrating surface water. Fluid evolution can be studied indirectly by detecting signs of water-rock interaction in matrix minerals and in fracture and vein fillings, and directly by measuring the chemical and isotopic compositions of fluids presently found in the interconnected pore space as well as in fluid inclusions in the target formation and its neighbours.

Water-rock reactions occur in all types of argillaceous media. It is important to distinguish between matrix and vein or fracture minerals, and among different generations of veins and fractures. Water-rock reactions at fracture boundaries can give natural evidence about the extent of matrix diffusion.

24.2 Site-specific experimental information

Formation/ site	Results and conclusions	Reference
Toarcian-Domerian at Tournemire	A number of pore-water tracers were investigated in vertical profiles across the formation. ^{2}H and Cl can be interpreted to represent diffusion profiles, even though the mathematical fits require different parameter sets for these tracers. Using D_e values for HTO measured in the laboratory and assuming seawater as the initial pore-water composition leads to build-up times for the diffusion profiles of *ca.* 50 Ma, which is unrealistic because the age of the embedding aquifers is 25 Ma at most. The discrepancy remains open at the present stage. Variations of water isotopes were also analysed in small-scale profiles around water-conducting fractures. A disturbance can be identified within 1 m away from the fractures, even though the profile is complex and does not allow a simple interpretation.	Moreau- Le Golvan (1997), Boisson *et al.* (1998), Patriarche (2001)
Opalinus Clay at Mont Terri	Modelling of pore-water chemistry at Mont Terri indicates equilibrium with carbonate, and sulphate minerals and exchangeable cation capacities of clay minerals observed in formation. Br/Cl, SO_4/Cl, $\delta^{34}S_{SO4}$, $\delta^{18}O_{SO4}$ of pore-water are similar to those of seawater (see also FEP 25). Stable water isotopes show the same, and in addition record diffusional exchange with surrounding fresh waters. Pore-water within the Opalinus Clay and the Jurensis Marls retained its initial seawater character until the Jura Uplift when circulation of meteoric water began in relatively permeable horizons just above and below. At that time, diffusive loss of helium and diffusive exchange of isotopic forms of water began between the *in situ* pore-water and the adjacent meteoric water. Characteristic diffusion profiles of a number of tracers developed and can be evaluated quantitatively. Cl content of the formation has dropped only about 40% from its initial seawater value, δ^2H and δ^{18}O values of the *in situ* pore-water have reached only 70% of the meteoric water values, and the He profile in the pore-waters is in secular equilibrium between *in situ* production and diffusive loss, a state which requires some 4 Ma to become established.	Thury & Bossart (1999), Pearson *et al.* (2003), Rübel *et al.* (2002)

Formation/ site	**Results and conclusions**	**Reference**
Opalinus Clay in the Zürcher Weinland	In contrast to Mont Terri, element and isotope ratios in pore-water in the Benken borehole do not reflect marine signatures. Vein minerals contain fluid inclusions with both very high and very low salinities compared to present-day pore-water, indicating that fluid evolution was more complex than at Mont Terri. Profiles of water isotopes, Cl and Cl isotopes across the formation are interpreted to be due to diffusional exchange with the underlying aquifer *ca.* over the last 1-2 Ma (Waber *et al.* 2001). The overlying regional Malm aquifer is heterogeneous and contains stagnant saline waters in the Benken borehole, such that exchange by diffusion with the Opalinus Clay is minor or absent. Diffusion constants derived from the evaluation of natural tracer profiles are consistent with laboratory measurements.	Nagra (2002)
Opalinus Clay in the Zürcher Weinland and at Mont Terri	C and O isotope data of vein carbonates from the Benken borehole indicate equilibrium with seawater at temperatures consistent with the burial history of surrounding units. Bedding-parallel veins in Benken core were formed at temperatures 25 to 50 degrees C higher than those at Mont Terri. At Mont Terri, a second period of mineralisation occurred, presumably during the Jura folding. This event led to the formation of celestite and barite in cross-cutting veins.	Waber & Schürch (1999)
	Both at Mont Terri and in Benken core, vein mineralisations are very infrequent and volumetrically insignificant (<<1 permil), even within faults and fractures. Together with the absence of wall-rock alterations along faults, this is taken as evidence for very limited water flow along these structures throughout geological evolution.	Nagra (2002)
Boom Clay at Mol	The composition of the solid and liquid phases of the Boom Clay suggest that the Boom Clay pore-water is in equilibrium with the clay. Early diagenetic processes in the Boom Clay, as a result of organic matter degradation, resulted in the precipitation of pyrite and carbonate concretions. No indications of important mineral dissolution/precipitation events during later diagenesis have been recognised in the Boom Clay.	Griffault *et al.* (1996), De Craen *et al.* (1999), De Craen (1998).
Boda Clay Formation at Mecsek	C and O stable isotopes and ^{14}C in vein carbonate minerals indicate the depths to which recent waters from the overlying formations have penetrated into the fractures.	
Mizunami Group at Tono	Water chemistry, exchangeable cation populations and mineral surface textures were observed. Spatial changes of these show that cation exchange and calcite dissolution are dominant factors controlling water chemistry.	Iwatsuki *et al.* (1995)

Formation/ site	**Results and conclusions**	**Reference**
Couche silteuse at Marcoule	Tracer profiles of Cl and Br across the formation show characteristic shapes that can be interpreted as diffusion profiles. A quantitative evaluation was attempted but is limited by the incomplete knowledge of initial and boundary conditions for the diffusion process. No obvious discrepancies between field-derived and laboratory diffusion coefficients were identified.	Vitart *et al.* (1999)
Palfris Formation at Wellenberg	Water-rock interactions were extensive during thrusting and Alpine metamorphism some 20 Ma b.p. The dominant process was pressure solution and re-precipitation in veins. These consist of several calcite generations, ankerite and minor quartz. The overall volume proportion of veins is very high (several %). Since the cessation of the orogenic processes, only minute amounts of calcite were precipitated in fractures. Other evidence of post-Alpine water-rock interactions, e.g. along the brittle faults that developed during regional uplift of the region, do not exist in the rocks. H and O isotope data and chemistry of highest salinity borehole samples suggest that the origin of the saline end member is fluid from last-stage Alpine metamorphism.	Nagra (1997), Mazurek (1999)
	A layering of water types was identified within the Palfris Formation. 1. The deeper parts of the formation contain a Na-Cl water, which is interpreted to represent 20 Ma old metamorphic water because it has characteristics very similar to fluids trapped in fluid inclusions in vein quartz and calcite. The water is saturated with methane, and it is possible that small amounts of free methane gas exist in the formation (again analogous to findings in fluid inclusions). 2. Towards shallower depths, a transition is identified to Na-HCO_3 waters which are explained as meteoric waters affected by ion exchange reactions. 3. Surface-near waters are of the Ca-HCO_3 type, with low mineralisation, representing young meteoric water. In summary, the deeper parts of the formation are thought to contain stagnant waters with ages of several Ma. At shallower levels, these waters are mixed with and diluted by surface-derived waters, which react with the rock by exchange on their way down.	Nagra (1997), Pearson *et al.* (1998)

With the exception of highly indurated and fractured host rocks (such as the Palfris Formation at Wellenberg or the Boda Clay Formation), there is very little or no indication at all in the rocks that water-rock interactions over and above those related to burial (recrystallisation, cementation; see FEP 53 for more details) occurred. This is a necessary (even though not always sufficient) argument to demonstrate that only limited flow occurred through the formations considered.

24.3 Scaling issues

Data are collected from core and other similarly small rock samples down the scale of single grains. The properties of matrix rock change slowly with space because of the slow rate of fluid and solute movement, so such small samples represent a relatively large volume of formation. Single grains are appropriate for study of water-rock reactions in fractures because the possibly more rapid flow in that environment may restrict equilibrium to minerals in direct contact with the fluid.

Tracer profiles across argillaceous formations can be used to upscale parameters measured in the laboratory, such as diffusion coefficients, provided the initial and boundary conditions for the tracer profile are reasonably well known. They also provide arguments on the (ir)relevance of advection, either along fractures or through the matrix.

24.4 Scientific level of understanding

The geochemical and isotopic reactions that lead to signatures of water-rock reactions are well understood. To interpret these signatures as observed in the rock may require additional information such as temperature/pressure at the time of reaction or the isotopic and chemical makeup of the reacting fluid.

24.5 Linked FEPs

Similarly to FEP 23, this FEP synthesises the interaction and the effects of most FEPs of the A (Undisturbed system) and C (Long-term evolution) groups.

24.6 Level of understanding from a PA perspective and treatment in PA

Information about fluid evolution provides evidence of diagenesis during past basin evolution. Knowledge of past and ongoing diagenesis will guide selection of the processes that should be considered in PA.

24.7 Available reviews

NEA (1993, 1999b).

24.8 Planned work

None reported.

24.9 Overall evaluation

Information on fluid evolution is based on re-interpretation from a slightly different perspective of data collected in response to other FEP s, as specified in Section II, Chapter 24.5. It is important that this re-interpretation be made to assure that relevant processes are considered in developing the PA strategy.

25. WATER RESIDENCE TIMES IN THE HOST FORMATION (FEP A3.3)

25.1 Definition and generalities

This FEP refers to water residence times in the host considered as an attribute of system understanding and as a tool to build confidence in predictive models. The term "residence time" in this context is the time during which an elementary volume or mass of water or solute has been within the formation. A macroscopic sample of water or solute is composed of many elementary units with a distribution of residence times. The residence time of the sample is the volume-weighted average of the residence times of the elements it contains (Bolin & Rodhe, 1972; Etcheverry and Perrochet, 1999, 2000). The FEP is relevant to the far field in connection with site characterisation and nuclide transport properties.

Residence times can be estimated from the hydraulic properties and flow geometry of the formation, from concentrations of isotopes associated with radioactive decay or production, or from stable isotopic or chemical indicators of the recharge conditions of the water or the origin of solutes. Confidence in the hydrodynamic process modelling used to support PA is increased if the residence times they predict are similar to those inferred from natural evidence.

It is necessary to distinguish among the residence times of water and various solutes. Their transport properties and origins may differ, and so may their residence times. They are likely to be estimated using different techniques and measurements.

25.2 Site-specific experimental information

The following site-specific information is based on the chemical and isotopic properties of water and solutes, interpreted in some cases using transport models:

Formation/site	Parameters measured	Residence time information	Reference
Toarcian-Domerian at Tournemire Fracture fluid	$^{2}H_{H2O}$, $^{18}O_{H2O}$	Results influenced by fracture-matrix interactions and not interpretable.	Ricard (1993), Moreau-Le Golvan (1997), Moreau-Le Golvan *et al.* (1997, 1998, 1999), Patriarche (2001)

Formation/site	Parameters measured	Residence time information	Reference
Opalinus Clay and adjacent argillaceous units at Mont Terri Matrix fluid	Br/Cl, SO_4/Cl, $\delta^{34}S_{SO4}$, $\delta\,^{18}O_{SO4}$	Characteristic of depositional seawater.	Thury & Bossart (1999)
	He (^{4}He / ^{3}He)	*In situ* production coupled with out-diffusion.	Rübel *et al.* (2002)
	$^2H_{H2O}$, $^{18}O_{H2O}$	Characteristic of depositional seawater until diffusive exchange with bounding fresh water began.	Rübel *et al.* (2002)
Opalinus Clay in the Zürcher Weinland Matrix fluid	$^2H_{H2O}$, $^{18}O_{H2O}$	Shifted to the right of the GMWL, indicating very long residence times.	Nagra (2002)
	$^2H_{H2O}$, $^{18}O_{H2O}$, Cl	Vertical trends of these tracers are interpretable as diffusion profiles with build-up times of 0.5 - 2 Ma.	
Boom Clay at Mol Matrix fluid	$^{14}C_{TIC}$	Below detection.	Beaufays *et al.* (1994)
Mizunami Group at Tono Matrix fluid	$^2H_{H2O}$, $^{18}O_{H2O}$	Recharge temperature lower than at present.	Mizutani *et al.* (1992)
	$^3H_{H2O}$	Below detection; Residence time > 40 a.	
	$^{14}C_{TIC}$	Dilution corrected using ^{13}C; Residence time > 10 ka.	

25.3 Scaling issues

All data are based on point samples (borehole or core samples). Because of generally long residence times (due to diffusional transport only) matrix fluid changes occur only slowly with time or distance, and data are often interpreted using transport models representing full formation thickness. The essential correctness of this approach is illustrated by the regular shapes of tracer concentrations or ratios ("diffusion profiles" of Cl, ^{37}Cl, $^2H_{H2O}$, $^{18}O_{H2O}$, He, *etc.* in Opalinus Clay both in the Benken borehole and at Mont Terri, Callovo-Oxfordian at Bure, Toarcian-Domerian at Tournemire, Couche silteuse in Gard). Fracture fluid flow may be more rapid so fluid properties may change more quickly with time and distance and may not be representative of adjacent matrix fluid.

25.4 Scientific level of understanding

There is broad understanding and experience in the use of chemical and isotopic indicators of residence times. Their successful application requires collateral geochemical and hydrogeological information, on boundary conditions, for example, that may not always be available.

Samples from fractures are likely to represent mixtures of fluids moving through various sets of fractures and between fracture and matrix pore fluids. Interpreting the age of mixtures from their isotopic properties requires knowledge of the mixing ratios of component fluids. This may be available from chemical indicators of mixing or from concentrations of several environmental radioisotopes of different half-lives, but is generally not possible.

25.5 Linked FEPs

Interpretation of residence times from isotope and chemical data requires consideration of:

FEP 17	Pore- and fracture water composition
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 50	Past burial history

25.6 Level of understanding from a PA perspective and treatment in PA

Residence times from environmental isotope and solute composition data: (1) improve system understanding and (2) can be used to check the results of hydrodynamic models (whose results are then used in PA models).

25.7 Available reviews

There are no general reviews of residence time determinations in pore-waters of argillaceous formations. The applications of environmental isotopes in hydrogeology, including their use for determining residence times are described in the textbook by Clark & Fritz (1997). The discussion of the noble gas work at Mont Terri includes general background on the topic and additional references (Pearson *et al.*, 2003, Annex 5). Proceedings of a NEA workshop on “Use of Hydrogeochemical Information in Testing Ground-water Flow Models” provide, a broad summary and examples of this topic (NEA, 1999b).

25.8 Planned work

The PHYMOL project, a study of the palaeo-hydrogeology of the Mol site, includes environmental isotope and noble gas analyses (Marivoet *et al.*, 2000). It focuses mainly on the surrounding aquifers.

25.9 Overall evaluation

Residence time determinations may not be possible in all systems. However, if they can be found, they provide additional information on retardation mechanisms and flow rates. Corroboration of residence times calculated using transport models adds confidence to flow modelling.

26. OXIDATION OF THE HOST ROCK (FEP B1.1)

26.1 Definition and generalities

During repository operation and following closure, transient oxidising conditions will be encountered from oxygen in air introduced during operations. They could have a large effect upon redox potential and pH and thus on solubility limitation of radionuclide concentrations and the corrosion of the inner steel overpack, and could cause mineralogical changes in the host rock. Radiolysis of water in the immediate environment of waste packages (especially for high-level waste) can also produce species such as free hydrogen and oxygen influencing the redox potential. This FEP refers only to mineralogical changes in the host rock. It is particularly relevant to pyrite-bearing formations, but the process can also affect organic material and other Fe+2-bearing minerals. This FEP is relevant to the affected field in connection with the EDZ.

Oxidation of pyrite may lead to the precipitation of new phases such as Fe(OH)3. The sorption capacity of this phase, when freshly-precipitated, may be high and it can act to retard the movement of radionuclides through the affected field into the host formation (see FEP 21). Because all formations considered (except London Clay) contain carbonate, pH is buffered by calcite dissolution, and acidic conditions are not expected to develop at any time.

26.2 Site-specific experimental information

The argillaceous formations considered (except for the Boda Clay Formation) were deposited under reducing conditions, which were preserved until the present. Solids controlling redox conditions include sulphides (mainly pyrite), carbonates (siderite, ankerite) and organic matter. Whereas the partial oxidation of pyrite may occur rapidly in many of the formations (e.g. Boom Clay, Opalinus Clay, Oxford Clay, Toarcian-Domerian at Tournemire, Callovo-Oxfordian at Bure), effects on carbonates have not been reported, either because they do not occur or because they were not looked at. Oxidation of organic matter appears to be very slow in comparison to the time scales of exposure during repository operation. Acid waters associated with sulphide oxidation (known from mining dumps, acid mine drainage) do not occur in the formations considered here because they all contain sufficient quantities of carbonate to buffer pH.

Formation/ site	**Results and conclusions**
Toarcian-Domerian at Tournemire	EDZs of two different ages (*ca.* 100 a and *ca.* 10 a) were studied. The extent of pyrite oxidation is very limited, and products include gypsum, Fe-oxi-hydroxides, celestite and jarosite. Alteration rims in the adjacent rock matrix are absent. Regarding oxidation, there are no major differences between the two EDZs (Charpentier 2001, Charpentier *et al.* 2001).
Opalinus Clay in northern Switzerland	A number of field, microscopic and geochemical observations on the Opalinus Clay have been made (Mäder & Mazurek 1998, Mäder 2002). Observations at Mont Terri show that gypsum forms on some EDZ fracture surfaces within months to years after tunnel excavation, but there is no obvious associated deterioration of rock quality. Pyrite is the only significant phase to undergo oxidation in the Opalinus Clay, and mass balance arguments associate the sulphate source for the gypsum observed with pyrite oxidation. Acid production is buffered by calcite dissolution, so no acid plume is noted. Reaction products include gypsum, jarosite (rarely) and ferric hydroxides. Observations and microscopic and geochemical studies in the EDZ of a 150 y old tunnel penetrating Opalinus Clay, and in open pits and outcrops exposed at least thousands of years, describe pyrite oxidation over longer times. At times from tens to hundreds of years, visible brown oxidation zones (5-10 mm) bordering EDZ fractures are evident, with <25% of pyrite oxidised. Penetrative oxidation, some with significant sulphate mass transfer, is found at times of thousands of years and more. Observations on some laboratory experiments using Opalinus Clay suggest the possibility of very rapid pyrite oxidation and visible rusty discoloration of pyrite after weeks. The occurrence of what seem to be anomalously high sulphate concentrations in some waters from squeezing and leaching experiments is attributed to pyrite oxidation during core sample collection, storage and preparation for analysis (Pearson *et al.*, 2003, ch. 4.3).
Boom Clay at Mol	The CERBERUS test (Control Experiment with Radiation of the Belgian Repository for Underground Storage) simulated the irradiation and thermal effects of a Cogema high-level waste canister after 50 years cooling time. During the 5 year test, clay in contact with the canister wall was submitted to dose rates up to 400 Gy/h, with total absorbed doses reaching 17 MGy. The temperature was ~ 100°C. Post irradiation studies were performed on Boom Clay host rock and engineered barriers samples (Noynaert *et al.*, 1998b). The main conclusions were that the radiation exposure did not unfavourably change the geochemical conditions of Boom Clay, which remained strongly reducing and nearly neutral around Cerberus. This could be due to the good buffer capacity of the Boom Clay itself or the chemical protection of the hydrogen formed by radiolysis in the pore-water surrounding Cerberus. Thus hydrogen escapes from the system slowly because of its control by diffusion only. The interstitial clay water changes progressively from a sodium bicarbonate type to a sodium sulphate type, due to oxidation of pyrite induced by the radiation and heating fields. The heat and radiation around the Cerberus test do not induce large mineralogical changes. The mineralogy of clay minerals remains nearly unchanged as shown by XRD analysis. No illitisation was observed.

Formation/ site	Results and conclusions
	Modelling has been done to evaluate the transient oxidising period after closure of a hypothetical repository in the Boom Clay considering oxygen in the pore-water and the bulk amount of iron consumed in the corrosion of the overpacks of vitrified high-level waste (Einchcomb & Grindrod 1995). Reaction with the carbon steel resulted in aerobic conditions with the corrosion rate limited by diffusive transport of oxygen towards the steel-bentonite interface, diffusion of the corrosion products outward from the buffer into the surrounding Boom Clay and reaction with ambient minerals (e.g. pyrite). The maximum duration of the anaerobic corrosion phase is 11 years. Including diffusion into the surrounding Boom Clay and pyrite oxidation in the Boom Clay reduces this to as little as 3.1 years, depending on the rate of pyrite oxidation.

26.3 Scaling issues

The distance scale of the Opalinus Clay observations is micrometres to metres and is appropriate to PA. The time scale is weeks to hundreds of years and is appropriate for the operational phase.

26.4 Scientific level of understanding

Experience with the Opalinus and Boom Clays suggests that only pyrite is susceptible to oxidation over the time scales of interest. The chemistry of pyrite oxidation (and the possible oxidation of other reduced substances in these formation such as organic C, and Fe^{+2} or Mn^{+2} bearing minerals) is well understood in theory (Pearson *et al.*, 2003, ch. 5.2.3, Rimstidt & Vaughan, 2003). The kinetics of pyrite oxidation are not well known, but constraints based on mass balance and oxygen diffusion rates are likely to be provide at least upper bounds on the extent of host rock oxidation.

26.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 15	Natural organics, complexation
FEP 17	Pore- and fracture water composition
FEP 18	Dissolution / precipitation of solid phases
FEP 22	Thermodynamic and kinetic modelling data
FEP 27	Redox buffering capacity of the host rock
FEP 31	Thermal effects on mineral stability and pore-water composition
FEP 35	Size and structure of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 45	Gas dissolution and chemical interactions between gas and pore-water
FEP 49	Microbiological perturbations
FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)

26.6 Level of understanding from a PA perspective and treatment in PA

Observations in the Boom and Opalinus Clays suggest that while oxidation effects may be evident, they are spatially very restricted and modify neither the geochemical (redox) state nor the physical properties of the formations. Thus, they are not included in PA analyses.

26.7 Available reviews

The influence of redox reactions on pore-water chemistry is covered in most textbooks of aqueous geochemistry and by Pearson *et al.* (2003, ch. 5.2.3). The results of the radiation-effects experiment at Mol are given by Noynaert *et al.* (1998b), and the observations and conclusions on the Opalinus Clay and Palfris Formation by Mäder & Mazurek (1998) and Mäder (2002).

26.8 Planned work

Some oxidation of the Boom Clay has been observed during the excavation of the connection gallery in 2002. A report is in preparation and is expected to be published in 2003.

26.9 Overall evaluation

Oxidation of the host rock induced by ventilation of the repository during the operational phase or by irradiation is well understood and its importance to the PA of a given site or repository configuration can be determined in each case. This conclusion relies mainly on experimental, *in situ*, natural analogue and modelling data for the Boom Clay and Opalinus Clay.

27. REDOX BUFFERING CAPACITY OF THE HOST ROCK (FEP B1.1.1)

27.1 Definition and generalities

The redox buffer capacity of a system is a measure of its ability to resist changes in the redox potential. To be fully analogous to the widely used pH buffer capacity, the redox capacity would be defined at a given Eh as the quantity of strong oxidant that, if added to 1 litre of sample, would raise the Eh by one volt. The terms oxidative capacity (**OXC**) and reductive capacity (**RDC**) were defined by Scott & Morgan (1990):

$$\mathbf{OXC = \Sigma\, n_i\, [Ox]_i - \Sigma\, n_i\, [Red]_i = -RDC}$$

where $\mathbf{[Ox]_i}$ and $\mathbf{[Red]_i}$ are the concentrations of individual oxidants and reductants and $\mathbf{n_i}$ is the number of electrons transferred in each redox couple reaction. **OXC** and **RDC** values for a system are determined by titrating the system with a strong oxidant or reductant, respectively. Redox capacity values defined this way are similar to the total acid or base consuming capacity of a system.

The ability to resist oxidation depends on values of $\mathbf{[Red]_i}$, the concentration of substances such as sulphide and elemental sulphur, ammonium, organic carbon, and ferrous iron and other reduced metals. The capacity to resist reduction depends values of $\mathbf{[Ox]_i}$, the concentrations of substances such as dissolved oxygen, nitrate, sulphate, and ferric iron and other oxidised metals. Heron & Christensen (1994) define the total reduction capacity (**TRC**) of a formation based on its concentrations of species that can be readily oxidised (reduced manganese, reduced iron, oxidisable organic carbon, reduced sulphur and reduced nitrogen) as:

$$\mathbf{TRC = 2\,[Mn^{2+}] + [Fe^{2+}] + 4\,[COOx] + 8\,[S^{2-}] + 7\,[HS^{-}] + 8\,[NH_4^{+}]}$$

which is an explicit formulation of Scott & Morgan’s expression above.

Substances oxidise at different oxidation potentials, and some substances can be oxidised only slowly. Thus the concept of an *effective* rather than a *total* redox capacity may be more useful. The effective redox capacity would include only those substances that would oxidise within the range of redox potentials of interest and at a rate commensurate with the time periods of interest.

27.2 Site-specific experimental information

The redox buffer capacity of the pore-water of Opalinus Clay at Mont Terri is negligible, but one kg pore-water *in situ* is associated with about 38 kg rock, so the redox capacity of the system is dominated by that of the rock. The total reduction capacity of the Opalinus Clay at Mont Terri ranges from 2.3 to 4.9 meq/g, based on chemical analyses of 7 core samples. Titration of one sample with $K_2Cr_2O_7$ gave 4.8 meq/g, in good agreement with the values from the nearest analysed cores (Gaucher *et al.*, 2003).

Mäder (2002) examined evidence of oxidation in exposures of Opalinus Clay and Palfris Formation in tunnels, quarries and outcrops (see FEP 26). From these, he concludes that only pyrite oxidation is likely to occur over the time scale of repository operation. Thus, the *effective* reduction capacity of the Opalinus Clay is due to pyrite alone and is only 0.1 to 0.2 meq/g, far lower than the *total* reduction capacity of the formation. The remaining reduction capacity is due to siderite and organic C and, if available at all, would be felt only on very long time scales.

The redox buffer capacity of the Boom Clay at Mol is 2 meq/g.

27.3 Scaling issues

The redox capacity of host formations will not vary spatially, except for clusters of pyrite crystals, so scaling is not an issue.

27.4 Scientific level of understanding

The equilibrium chemistry of redox buffering is well understood. However, the rates at which various oxidation-buffering reactions may take place are not well known and may require site-specific evaluation.

27.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 15	Natural organics, complexation
FEP 18	Dissolution/precipitation of solid phases

27.6 Level of understanding from a PA perspective and treatment in PA

Nagra concludes that canister corrosion products have a strong buffering capacity for radiolytic oxidants. In addition, pyrite and siderite in the bentonite could act as reductants (Johnson & Smith, 2000). For this reason Nagra does not take into account the redox buffering capacity of the Opalinus Clay in a safety assessment base case (only for *what if* scenarios).

In some other programmes, oxidation processes are treated indirectly by demonstrating that the depth penetration of the effects into the host formation is limited. For PA calculations, the length of the flow path is reduced by the size of the zone affected by oxidation.

27.7 Available reviews

Redox reactions in natural waters are discussed in any textbook of aqueous geochemistry. Stumm & Morgan (1996) provide particularly useful discussions of the potentials at which various redox reactions occur and of the rates of redox reactions. Langmuir (1997), in addition, discusses definitions of redox capacities and the analogies between pH and Eh buffer capacities and strengths.

27.8 Planned work

None reported.

27.9 Overall evaluation

The importance of this FEP in PA is likely to be scenario dependent. It is not treated explicitly in most programmes.

28. EFFECTS OF REPOSITORY COMPONENTS ON PORE-WATER CHEMISTRY IN THE HOST ROCK (FEP B1.2)

28.1 Definition and generalities

A repository will contain a number of substances foreign to the host rock such as iron and other metals used for tunnel construction and stabilisation, and for waste handling and protection, as well as bentonite buffer and backfill material. This FEP addresses the possible effects of this material on the chemistry of the host rock. It is relevant to the affected field in connection with the EDZ. Note that cements are excluded here and covered by FEP 29.

28.2 Site specific experimental information

None reported.

28.3 Scaling issues

None reported.

28.4 Scientific level of understanding

None reported.

28.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture water composition

28.6 Level of understanding from a PA perspective and treatment in PA

None reported.

28.7 Available reviews

None reported.

28.8 Planned work

None reported.

28.9 Overall evaluation

This FEP is not considered explicitly by any organisation, but it is implicit in considerations given other FEPs as discussed in Section II, Chapter 28.5. At least in diffusion-dominated systems, any effects would be expected to be spatially limited. Note that cement may also be present in repositories. The effects of cement are included in FEP 29 and are excluded from this FEP.

29. INTERACTION OF HYPERALKALINE FLUIDS AND HOST ROCK (FEP B1.2.1)

29.1 Definition and generalities

This FEP addresses the influence of hyperalkaline (pH > 10.5) fluids of high Na, K and/or Ca contents that may enter the formation (EDZ and beyond) and react with the host rock.

Hyperalkaline fluids could be produced by degradation of cement and concrete used in the construction of low and intermediate-level radioactive waste repositories for structural, encapsulation and backfilling purposes, or present in high level waste repositories as plugs or backfill. These interactions, consisting of ion exchange and mineral dissolution and precipitation reactions, may impact the performance of the repository by potentially changing sorption, ground-water flow, and matrix diffusion behaviour, *inter alia.* For repository safety assessment purposes, it is necessary to evaluate the type and magnitude of these interactions and their potential impact upon waste isolation.

The effects of this FEP on the performance of repositories in fractured rock may differ from its effects on those in unfractured rock. In both cases, it could cause physical and chemical changes in the bulk transport properties of the rock. In fractured rock, it could either increase or decrease fracture apertures, and, by dissolution or precipitation on fracture walls, could also affect solute exchange between matrix and fracture fluid and so modify the retardation expected from matrix diffusion.

29.2 Site-specific experimental information

Formation/ site	**Results and conclusions**
Opalinus Clay at Mont Terri	At Mont Terri, an *in situ* diffusion experiment, the CW-Experiment, was carried out in a packed-off test interval of 3.5 l volume, at 10 m depth, heated to 35 °C. The interval was kept at 11 bar pressure, 1-2 bar above pore-water pressure. The test interval was connected to a reservoir and mass flow into rock was monitored. The fluid was a K-Na-Ca-OH solution, at pH = 13.2, saturated with $Ca(OH)_2$, which was periodically replenished and analysed and has been circulated since March 2000. Overcoring of the test interval failed in October 2001. Initial results show that buffering to pH 10 took place over 6 months, but that subsequent buffering is less efficient. Mass loss to the rock is about 2 g/day, and no significant decrease of the mass transfer rate was observed (Mäder *et al.* 2000). No detailed chemical interpretations have yet been made nor any specific modelling efforts, but some work is carried out in the framework of ECOCLAY II, an EU 5th framework programme. Experiments at the Mont Terri underground research laboratory indicate a diffusion-dominated regime lacking fracture-controlled or other preferentially transmissive features except for the EDZ.

Formation/ site	**Results and conclusions**
Boom Clay at Mol	SCK•CEN performed *in situ* experiments on the reaction at the interface between Boom Clay and concretes of different types (waste conditioning concrete and construction concrete). These experiments did not provide data on pore-water chemistry changes but indicated that after 1 to 1.5 years of contact the mineral reaction zones both in the clay and in the concrete were limited to a very narrow zone of about 100 to 150 µm (Read *et al.*, 2001b).
Laboratory studies	Several laboratory studies with Opalinus Clay samples have been finalised or are in progress (see Nagra 2002). At the University of Bern, a high-pH infiltration experiment on a drill core sample of Opalinus Clay was performed at 50 bar confining pressure, a 30 bar constant head, at 30 °C, in a He atmosphere. Advective-dispersive piston flow was at a rate of 1/2 pore volume per week and decreased very slowly and steadily with time before dropping rapidly to zero after 14 months. The infiltrating fluid is a K-Na-Ca-OH type at pH=13.2, saturated with $Ca(OH)_2$. The effluent was still buffered at pH = 9.6 after 14 months of infiltration (Adler *et al.*, 2001, Nagra, 2002, ch. 7.5). The results show that the high-pH plume infiltrating the rock is effectively buffered for the entire duration of the experiment by the combined process of displacement of Mg from the ion exchange complex, dolomite dissolution and precipitation of Mg-hydroxide phases. Significant precipitation of secondary calcite and illitic clay continuously reduce the hydraulic conductivity and require the dissolution of primary silicates such as kaolinite and quartz. It is not straightforward to interpret the observed final drop to zero-flow – either a completely impermeable zone within the rock matrix was produced or some phenomenon like a significant entry pressure to drive flow is implied. High-pH diffusion and advection scoping experiments on samples of Opalinus Clay have also been carried out using a K-Na-Ca-OH fluid of pH=13.2, saturated with $Ca(OH)_2$. Secondary minerals were detectable after 2-4 weeks at ambient conditions. A schematic time evolution of alteration sequences has been derived. Different parageneses were observed in diffusion and advection experiments. The diffusive regime is a more efficient buffer and promotes zeolite formation while the advective regime generates C-S-H type phases near the inlet. There is evidence for preferential flow paths at a microscale, but overall front propagation is homogeneous (Adler *et al.* 1999). High-pH column experiments were carried out by BGS on pure minerals and crushed rocks, including marl of the Palfris Formation. Flow-through columns were used with Ca-OH and K-Na-Ca-OH solution at 70°C. Extensive formation of C-S-H phases was noted as well as extensive clogging of flow paths within months. (Bateman *et al.*, 1997, 2000). In the framework of the ECOCLAY II project, laboratory experiments with bentonite/clay plugs are running and it is planned to start new experiments, including *in situ* tests, on the influence of concrete water on the pore-water chemistry in the EDZ (e.g. partial pressure of CO_2).

Formation/ site	**Results and conclusions**
Modelling	Reactive transport modelling of high-pH fluid-rock interaction has been reported based on a simple fracture / rock matrix (dual porosity) system. The modelling used parameters relevant to the Maqarin Natural Analogue Site, specifically for the rock matrix. The role of dolomite dissolution to promote calcite precipitation is a crucial factor in the sealing tendency of rock matrix adjacent to fracture pathways (Steefel and Lichtner 1994, 1998a, 1998b). A reactive transport model was constructed for the core infiltration experiment using an Opalinus Clay sample mentioned above, combining advection, dispersion, ion-exchange and mineral reactions (Adler 2001, Adler *et al.* 2001). It was possible to match the observed effluent chemistry with a combination of independently constrained parameters and a limited number of fit parameters. Some details of the model were transferred to a pure diffusion case and are summarised in Nagra (2002, ch. 7.5). IRSN, in collaboration with French School of Mines (ENSMP-CIG), developed the HITECH coupled code, which is suited to quantify hyperalkaline effects. The chemical interactions between industrial materials and the host rock are modelled with the reactive transport code HYTEC for time scales and geometries representative of disposal projects (De Windt *et al.*, 2001a, b). The pH evolution, a key parameter in element mobility, is studied more specifically. It depends on several interdependent processes: i) diffusion of highly alkaline cement pore solution, ii) strong buffering related to major mineral transformations both in the cement and in the clay, and iii) cation exchange processes beyond the zone of intense mineral transformations. In addition, precipitation of secondary minerals may lead to a partial or complete clogging of the pore space, thus limiting the propagation of the high-pH plume. Research is ongoing to better assess the effect of geochemical processes on hydrogeology and on porosity changes, notably to understand the importance of kinetics and of fractures in the EDZ. Models combining radionuclide migration and cement-clay interactions are developed in parallel.

Formation/ site	Results and conclusions
Natural analogues: Maqarin and Kusheim Matruk (Jordan)	Observations at the Maqarin Natural Analogue Project (Jordan) indicate that the rock matrix adjacent to fracture-controlled pathways has been affected (mm to cm). Although the clay-mineral content is low, clay-mineral alteration is observed. The pH is buffered at high values (12.5-12.8) along tens to hundreds of m of flowpath by C-S-H phases. Stages of alteration product assemblages are identified in fractures and adjacent rock matrix, and secondary mineral assemblages are comparable (Smellie *et al.* 1997, Alexander 1995a, b, Linklater *et al.* 1996, Linklater 1998, Smellie 1998). Another important observation is that the consequence of the recurrent stages of fracture reactivation (probably due to slumping of the steep hillslope and/or tectonic activity) and subsequent percolation of hyperalkaline water is always fracture sealing by reaction products. This means that the rate of rock-matrix dissolution is lower than the rate of precipitation of alteration products in the fractures. This observation stands against some earlier model calculations which predict major dissolution and enhancement of fracture apertures. These calculations were made using unrealistic boundary conditions and also neglected precipitation in the fractures (Steefel & Lichtner 1994). A new natural analogue study has begun in Kusheim Matruk, Central Jordan, on a fossil hyperalkaline system adjacent to rocks with more clay minerals (10-30%) than at Maqarin. Preliminary studies document clay-mineral alteration, but only progress reports are yet available (Smellie *et al.* 2000). One of the major problems at this site is the difficulty to distinguish the effects of contact metamorphism and hyperalkaline alteration on clay minerals and other constituents. Veins and alterations possibly attributable to hyperalkaline effects are rare and occur only within about half a metre away from the cement zone. The temperature at which potential interactions with hyperalkaline interactions occurred (possibly during the cooling stage of the metamorphic body?) is not constrained, and this limits the applicability of this site as a natural analogue.

29.3 Scaling issues

The distance scale is mm to cm for laboratory experiments and mm to tens to hundreds of m for natural analogues, which are relevant to PA. The time scale is too short in experiments but appropriate in natural analogues. Scaling of time is problematic due to large uncertainties in reaction rates at high-pH. Over long periods of time reaction rates are less crucial due to the approach to (dynamic) equilibrium.

29.4 Scientific level of understanding

The process is understood qualitatively in unfractured argillaceous rock, but quantitative understanding is not sufficiently advanced yet to perform numerical predictions. The tendencies of system evolution are understood sufficiently to allow for qualitative extrapolation, but quantitative extrapolation is not yet reliable.

Modelling reactions of hyperalkaline fluids is made particularly uncertain by the poorly defined physical properties, chemistry, and thermodynamic and kinetic constants of the variety of solid phases that may form (gels *vs.* crystalline solids, solid solutions).

29.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 6	Hydraulic properties of the host rock
FEP 8	Diffusivity
FEP 9	Connected matrix porosity
FEP 12	Colloid formation, transport and filtration
FEP 13	Flow-wetted surface and accessibility of matrix
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 18	Dissolution/precipitation of solid phases
FEP 19	Solid solutions/co-precipitation
FEP 20	Ion exchange
FEP 21	Surface complexation
FEP 22	Thermodynamic and kinetic modelling data
FEP 35	Size and structure of the EDZ
FEP 38	Hydraulic properties of the EDZ
FEP 42	Self-sealing

29.6 Understanding from a PA perspective and treatment in PA

This FEP may be treated implicitly through the assessment of the radionuclide solubility and the effective thickness of the argillaceous barrier. In some programmes, this FEP is treated solely by reducing the length of the flow path through the formation by the size of the zone affected by hyperalkaline effects. This size can be shown to be very limited in diffusion-dominated systems but is less straightforward to estimate in fractured, potentially advection-dominated formations.

29.7 Available reviews

General radwaste-related reviews include Smellie *et al.* (1997) and Alexander (1995b).

29.8 Planned work

Continuing and additional work is planned or ongoing both at Mol and at Mont Terri.

Work at Mol is carried out in part under ECOCLAY II in the EU 5th Framework programme. Experimental work includes: percolation and diffusion tests on cores, first with non- or poorly sorbed radionuclides and later with strongly sorbed elements; a test is expected to be performed *in situ* in the underground research laboratory in order to evaluate the impact of this process under real conditions. A continuous influx of bicarbonate ions from the surrounding argillaceous formation might significantly restrict the progression of the alkaline plume and limit its impact to the vicinity of the repository (diffusion of bicarbonate ions and neutralisation of the plume before it reaches the far field). Modelling work includes review and formulation of mineral precipitation and dissolution models, suggestion of alternative experimental designs; scoping calculations for percolation and diffusion experiments (blind predictions) and evaluation and calibration of models based upon experimental data. The time scale should be around 4-5 years starting from 1999 (possible *in situ* test not included). An extension of the programme is highly probable.

Modelling work on Opalinus Clay continues in the framework of ECOCLAY II, It is planned to extend the model of Adler (2001) to longer time scales assuming pure diffusion and rock properties derived from samples from the Benken borehole.

29.9 Overall evaluation

This FEP is relevant to PA, but to make a full PA analysis further information is required. The main open issue is the influence on migration parameters, but further knowledge of properties required for geochemical modelling is also necessary. Given the fact that highly sorbing phases are precipitated due to the interaction of rock with hyperalkaline fluids, the overall effect on retardation is most likely positive, even though difficult to quantify with confidence at the present stage.

30. ORGANICS FROM WASTE AND THEIR EFFECT ON TRANSPORT PROPERTIES OF THE HOST ROCK (FEP B1.2.2)

30.1 Definition and generalities

Organics from waste include different types of organic substances that are found in radioactive waste products and waste matrices. They may be leached or degraded both from material in which radioactive waste is embedded (e.g. compacted and cemented cellulose-based waste, resins, plastics, organic decontamination agents) as well as from waste encapsulating matrix material (e.g. bitumen in bituminised waste products, modifiers that influence the rheological properties of mortar used to produce cemented waste). Organics from waste are formed either as unaltered leaching products or as radiolytical, chemical and/or microbial degradation products that are generated according to waste- and repository-specific decomposition rates. Organics that originate from leaching or decomposition reactions, like those naturally present in the host rock and pore-water (FEP 15), may adsorb onto solid phases, precipitate, form complexes with radionuclides, and/or migrate in complexed or uncomplexed form in the affected and far field. Note that the use of organic materials in construction materials of the repository galleries (e.g. modifiers in the mortar for the concrete linings) will also result in the release of organics with properties and fates similar to those originating from the waste.

Potential effects of organics on transport through the host rock include

- Interactions with clay minerals (shrinkage, collapse, swelling), with resulting effects on hydraulic properties;
- Complexation of solutes on dissolved organic complexes or colloids, with effects on retention properties of the argillaceous formation.

30.2 Site-specific experimental information

Formation/ site	Type of information	Scale	Results and conclusions
Boom Clay at Mol	Organic waste degradation experiments; solubility and sorption tests with Pu(IV) and Am(III)	cm	Generation of potentially complexing agents such as ISA and oxalic acid (Valcke *et al.*, 1999a). Bitumen degradation products and ISA increase solubility (factor 4 to 15), but only weak influence on sorption.
London Clay	Sorption test to study influence of organic-matter degradation products on U(IV), Th(IV), Sn, Ra Themodynamic modelling	mm to cm	Sorption of U(VI), U(IV) and Th onto London Clay in the presence of gluconate and authentic degradation product cellulose leachates shows variable reduction in sorption. The experiments were performed at both neutral and high pH (Baston *et al.*, 1991, 2001).

Organic ligands – either naturally occurring or from the dissolution or degradation of materials introduced into a repository – can form complexes with certain waste radionuclides. Such complexing could:

- increase radionuclide solubility;
- decrease sorption, if the organics are not themselves sorbed;
- increase sorption, if the organics themselves are sorbed;
- decrease the rate of transport, if the size of organic complexes is sufficient to decrease their diffusion coefficients or increase their osmotic efficiencies;
- increase the rate of advective transport in fractures, for example, if the complex sizes are sufficient to decrease their effective transport porosity.

30.3 Scaling issues

None reported.

30.4 Scientific level of understanding

The decomposition of organic waste and bitumen matrix includes quite complex processes that are not fully understood. In the framework of nuclear waste disposal, the chemical effects of waste-derived organics on the properties of argillaceous formations are almost not studied.

From studies on the use of clay barriers for municipal and industrial (non-radioactive) waste disposal, it is well-known that organics can cause the collapse, shrinkage and cracking of swelling clay barriers made of bentonite (Rowe *et al.*, 1995). Although such effects have not been reported for natural argillaceous formations, this point is included as a reminder that they should not be overlooked in site characterisation and PA activities.

30.5 Linked FEPs

FEP 12	Colloid formation, transport and filtration
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 15	Natural organics, complexation
FEP 17	Pore- and fracture water composition
FEP 20	Ion exchange
FEP 21	Surface complexation
FEP 22	Thermodynamic and kinetic modelling data
FEP 41	Swelling
FEP 42	Self-sealing

30.6 Level of understanding from a PA perspective and treatment in PA

Effects on clay minerals are not expected to be relevant for high-level and most medium-level waste types. These waste types generally contain only small quantities of degradable organics, and measurements show that their influence is often weak. However, the foundation for this judgement is weak and should be improved. The principles of organic complexation are generally well understood and the effect of pure and/or synthetic organics is rather well known. Complexation with natural organics or organics from degradation products is however much more complex. Often there is only little knowledge about the influence of the organics on sorption and thus mobility of the radionuclides.

Currently understanding of the influence on retardation allows only conservative treatment in PA by assuming higher solubility and lower sorption for radionuclides that are known to be easily complexed. Sensitivity and uncertainty studies are performed to assess the potential importance. There is little understanding of effects on hydraulic properties, and they are not considered in PA.

The relevance of this FEP varies among different disposal concepts, waste forms and the presence and nature of organics therein.

30.7 Available reviews

None reported.

30.8 Planned work

At SCK•CEN, further work on organics from bitumenised medium-level waste is foreseen. Further experimental work connected with PA concerning the influence of organics on solubility and sorption (mobility) of radionuclides is planned.

30.9 Overall evaluation

This FEP is poorly studied. Only wastes containing substantial quantities of organics such as cellulose or waste embedded in bitumen are expected to have significant effects. Current knowledge allows only conservative treatment in PA. Some organisations consider this FEP to be irrelevant, others have little information and are not able to assess the relevance. Of particular interest is the potential increase of solubility and mobility of some radionuclides. Experimental studies carried out till now indicate only a very moderate effects. For special waste types with large quantities of organics, further studies are planned to substantiate this conclusion. Effects of organics on hydraulic properties are expected to be negligible and are not considered.

31. THERMAL EFFECTS ON MINERAL STABILITY AND PORE-WATER COMPOSITION (FEP B2.1)

31.1 Definition and generalities

The equilibrium positions of chemical reactions vary with temperature, as do reaction rates. Rising temperatures increase the solubility of most solids, decrease the solubilities of most gases and increase most reaction rates. Results of changing temperature could be modification of the chemistry of pore-water and/or of formation mineralogy. Thermal effects on clay minerals and organic materials are most prominent in argillaceous formations.

This FEP is relevant to the region in which thermal anomalies from the repository extend, although it will be most relevant to the region of highest temperatures in the affected field.

31.2 Site-specific experimental information

The influence of past thermal effects on a given formation can be evaluated from the identity and crystallinity of clay minerals, properties of organic material such as its vitrinite reflectance, and the identity, chemistry, fluid inclusion properties and stable isotopic properties of secondary minerals, particularly those in fractures and veins.

Intense thermal effects can be evaluated using argillaceous rocks found near volcanic intrusions as natural analogues (Miller *et al.*, 2000). According to Bouchet *et al.* (1999) and Pellegrini *et al.* (1999a, b, c), the findings at different analogue sites suggest a temperature of *ca.* 100°C below which the modifications to the host formation are expected to be minor.

In the Spanish Reference Clay in a Tertiary basin, dehydration of rock-forming gypsum is expected as a consequence of the thermal pulse.

Nagra (2002) explicitly examined thermal effects in the Opalinus Clay. For the planned high-level waste repository in the Zürcher Weinland, the development of the thermal pulse emanating from the heat-producing waste was quantified by Johnson *et al.* (2001). Over a period of max. 1 000 y, temperature at the interface of bentonite and Opalinus Clay will exceed 80°C with a maximum of 95°C in the (worst) case of MOX/UO_2 canisters. These temperatures are only slightly higher than the maximum temperature of *ca.* 85°C experienced by the formation during maximum burial (see FEP 50). At the time when the thermal pulse will occur, the repository system will not be fully saturated, so that water is expected to flow from the formation into the engineered barrier system (and not *vice versa*). The following processes related to the thermal pulse were taken into account (Nagra, 2002, Mazurek, 2002):

- thermal maturation of organic matter;
- illitisation of the illite/smectite mixed-layer phase;

- acceleration of oxidation reactions (see FEP 26);
- changes in pore-water chemistry.

The first three processes involve kinetics, the fourth process can be described by equilibrium thermodynamics and is reversible.

Given the short time scales involved and the small difference to temperatures already experienced by Opalinus Clay during burial, thermal effects on organic matter and clay minerals were shown to be negligible. Pyrite oxidation in Opalinus Clay is most likely limited by the rate of oxygen diffusion into the matrix (Mäder & Mazurek, 1998). The increased diffusion coefficient at 95°C results in an increase of oxidation rate by a factor 4, which is also negligible *vis-à-vis* the limited magnitude of this reaction (see also FEP 26). The pore-water chemistry will change towards higher pH (*ca.* 0.6 units) and higher P_{CO2} (less than 1 log unit). The water type remains the same, with only slight changes in ion concentrations. The only relevant mineral reaction is calcite dissolution, with negligible effects on porosity.

It was concluded that all thermal effects, even on the interface to the bentonite, are negligible. This finding from the Opalinus Clay may not be easily transferable to other formations, in specific to those which experienced substantially lower temperatures during maximum burial, such as the Boom Clay and the Spanish Reference Clay, or the Callovo-Oxfordian at Bure.

31.3 Scaling issues

None reported.

31.4 Scientific level of understanding

The processes by which changing thermal conditions will affect mineral and solution properties are well understood and can be evaluated by geochemical modelling. For such modelling to be reliable requires data on the temperature-dependence of mineral transformations and water-rock interactions. It also requires the assumption of equilibrium or data for modelling reaction kinetics. However, there are uncertainties in thermodynamic and kinetic data for many reactions (FEP 22). Chief among these reactions are those for transformations among clay minerals (Mazurek 2002).

31.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 15	Natural organics, complexation
FEP 17	Pore- and fracture water composition
FEP 18	Dissolution / precipitation of solid phases
FEP 20	Ion exchange
FEP 21	Surface complexation
FEP 22	Thermodynamic and kinetic modelling data
FEP 32	Thermal rock properties

FEP 50 Past burial history

31.6 Level of understanding from a PA perspective and treatment in PA

Processes referred to in this FEP are not explicitly included in PA models because they are thought not to be important. However, the effects of changing thermal conditions should be evaluated to be certain their effects on the retardation and other properties of the host rock are not sufficient to change the output of the PA modelling by any significant amount. It should be noticed that in most recent repository concepts the maximum temperature that is expected to occur in the affected field is less than 100°C.

31.7 Available reviews

An example of consideration of thermal effects as background for a PA can be found in Nagra (2002).

31.8 Planned work

None reported.

31.9 Overall evaluation

The processes described in this FEP are not likely to have a significant effect on host-rock behaviour. A brief examination making use of the expected thermal regime can confirm this for a given site.

32. THERMAL ROCK PROPERTIES (FEP B2.2)

32.1 Definition and generalities

The most important thermal rock properties include:

(1) Thermal conductivity K $[W \ast m^{-1} \ast {}^\circ C^{-1}]$

(2) Heat capacity C $[J \ast kg^{-1} \ast {}^\circ C^{-1}]$

(3) Specific heat C_p $[W \ast s \ast kg^{-1} \ast {}^\circ C^{-1}]$

(4) Coefficient of linear thermal expansion ε_t $[{}^\circ C^{-1}]$

(1) and (3) yields:

(5) Thermal diffusivity $k = K / (\rho \ast C_p)$ $[m^2/s]$ with ρ = rock density

K, ε_t and k may be anisotropic, predominantly depending on the rock-specific degree of bedding (parameters measured ⊥ [normal] and // [parallel] to bedding).

32.2 Site-specific experimental information

Formation/site	Results and conclusions
Callovo-Oxfordian at Bure	From laboratory tests: $K_{\perp} = 1.65$ $[W \ast m^{-1} \ast {}^\circ C^{-1}]$; $K_{//} / K_{\perp} = 1.27$; K decreases significantly with decreasing degree of saturation. $C = 756$ $[J \ast kg^{-1} \ast {}^\circ C^{-1}]$ at 20 °C with C = f (temperature).
Toarcian-Domerian at Tournemire (mainly not site-specific work by IRSN)	• Determination of the classical parameters K, C. • Laboratory investigations on thermal and hydraulic diffusion in argillaceous rocks under thermal loading. Evolution of thermal conductivity as a f(T). Thermal properties of argillaceous rocks under thermal-hydraulic-mechanical strain (Djeran 1991). • Laboratory investigations on possible creep of different plastic clays under thermal strain (Bonne *et al.* 1991, Norotte *et al.* 1992; Boisson *et al.* 1993).
Spanish Reference Clay in a Tertiary basin	$K = 1.06$ $[W \ast m^{-1} \ast {}^\circ C^{-1}]$; $C = 1117$ $[J \ast kg^{-1} \ast {}^\circ C^{-1}]$; $k = 4.73 \times 10^{-7}$ $[m^2/s]$ (Enresa 1999).

Formation/site	**Results and conclusions**

Opalinus Clay in the Zürcher Weinland (Nagra 2001)	Heat capacity C: rather uniform, 920 ± 80 [J $*$ kg^{-1} $*$ °C^{-1}].
	Thermal conductivity K: Negligible influence from confining pressure (σ_3 applied was 5, 10, 15 and 29 MPa).
	Depth 622 m of the Benken borehole (higher quartz content): $K_\perp = 1.79 \pm 0.16$; $K_{//} = 3.23 \pm 0.11$ [W / (m °C)].
	Depth 642 m of the Benken borehole (lower quartz content): $K_\perp = 1.26 \pm 0.11$; $K_{//} = 2.04 \pm 0.23$ [W / (m °C)].

Boom Clay at Mol	Results from a large-scale *in situ* heating experiment in a clay pit were consistent with those on clay core samples. Measured values for saturated Boom Clay samples: K = 1.69 [W / (m $*$ °C)]; C_p = 1440 [W $*$ s / (kg $*$ °C)]; ρ = 2000 [kg/m^3]; k = 5.9 x 10^{-7} [m^2/s].
Boda Clay Formation at Mecsek	• *In situ temperature measurements* in the 1 030-1 080 m deep underground research laboratory and in adjacent boreholes. Large-scale monitoring of the cooling-down (ventilation) and re-warming (after shut down of the ventilation) processes provided reliable data for numerical back-analysis (Dolexpert & ME-SCI 1998). A hybrid 2-D UDEC plus the BEM computer code was employed. Best fit was achieved when K = 2.0 [W $*$ m^{-1} $*$ °C^{-1}]. • *Laboratory measurements*: Determination of K on re-saturated samples. Resulting range: $1.6 < K < 2.5$ W / (m °C) at room temperature. $K_{//} / K_\perp \sim$ 1.15 to 1.30. Within the temperature range of 20 to 65 °C, the K-values increased approximately linearly by 20%. Eight measurements focussed on the dependence of K on water content, and 5 to 9% lower K values were found for desiccated samples. Thermal diffusivity: $0.5 \times 10^{-6} < k < 1.3 \times 10^{-6}$ [m^2/s], with no identifiable temperature dependence.
Mizunami Group at Tono	• *Literature survey* of Japanese data on K, C, *etc.* • *Laboratory investigations* on core samples with regard to the above parameters (JNC, 1999a).

The data refer to water-saturated samples unless specified otherwise.

32.3 Scaling issues

Heat transfer is well understood and can be easily extrapolated in space and time. Scaling issues are of no importance for C and Cp, however of potential importance for K, k and ε_t. Evidence from Mol and other sites indicates that due to the high degree of structural and material homogeneity of argillaceous rocks, the scale factor is close to unity. Scaling issues are of minor concern.

32.4 Scientific level of understanding

The scientific level of understanding is very good. The mechanism of heat transport relevant for argillaceous rock with very low hydraulic conductivity (< 10^{-13} m/s) is predominantly conduction. Heat convection due to fluid flow and radiation are mechanisms of minor or no importance. In comparison with the mechanical and hydraulic properties of the rock, the natural scatter of the thermal rock properties is rather small.

32.5 Linked FEPs

FEP 9 Connected matrix porosity

FEP 14 Lithology, mineralogy of rocks and fracture infills

32.6 Level of understanding from a PA perspective and treatment in PA

This FEP is well understood with regard to processes and parameters for quantitative treatment in PA. The most important application of thermal parameters is the heat produced by high-level waste, and is generally considered as an important factor in the safety evaluation.

Modelling of heat transport in argillaceous rocks is based on the mechanism of conduction (application of heat transfer equations). Radiation and convection are neglected. Heat capacity and conductivity are used as input parameters for the calculation of the temperature evolution of a repository. The data have a direct implication on the layout of the repository (Johnson *et al.*, 2001). Within the conceptual model used for the Spanish PA, it is assumed that the thermal properties of the engineered barrier system (bentonite backfill) depend on the water content. For the host rock, however, thermal properties are assumed to be constant in time and independent of the water content and temperature (Enresa, 1999). SCK•CEN conclude that the impact of heat is rather limited as long as the container or overpack will prevent that ground water will come into contact with the waste during the thermal phase of the repository.

32.7 Available reviews

Site specific reviews: Spanish Reference Clay: Enresa (1999); Callovo-Oxfordian at Bure: AGEM (1998); Boom Clay: Put & Henrion (1992).

32.8 Planned work

Callovo-Oxfordian at Bure: Some heating tests aiming at characterising the THM response of the host rock will be carried out in the underground research laboratory. Site-specific thermal properties will be used in predictive modelling of the temperature distribution. The parameters will be checked by comparison of the numerical predictions with *in situ* measurements.

32.9 Overall evaluation

The temperature of the host rock formation in space and time depends predominantly on the specific thermal properties of the rock and on the heat generation rate of the high-level waste in the emplacement tunnel. The mechanical, hydraulic and chemical effects in the host rock which are associated with temporarily increased temperatures are important for the evaluation of the repository system particularly in the affected field with regard to the behaviour of the EDZ and the engineered barrier systems.

The site-specific thermal rock parameters have to be determined in line with established testing procedures, either in the laboratory and/or *in situ*. They represent indispensable input parameters for the analytical sections of a PA.

It is generally felt that the principal features of this FEP are sufficiently well understood. At this point in time no further work seems to be justified to enhance the scientific understanding of this FEP beyond current levels.

33. THERMALLY INDUCED CONSOLIDATION OF HOST ROCK (FEP B2.3)

33.1 Definition and generalities

The term “thermally-induced consolidation” relates on one hand to a radioactive heat source which is located in the backfilled emplacement tunnel (see also FEP 40) and, on the other hand, to a time-dependent solid-water interaction of cohesive materials (see also FEP 58). The time span over which the waste-derived heat pulse will act is of the order of some 1 000 to 10 000 years.

Subjecting a saturated cohesive material, such as a saturated argillaceous rock, to a temperature increase leads to a consolidation process which is similar to conventional mechanical consolidation (thermal stress instead of mechanical stress; Paaswell, 1967; Virdi and Keedwell, 1988). Initial thermal loading leads to a significant, irreversible consolidation which is manifested in a decrease of the void ratio (Campanella and Mitchell, 1968; Plum and Esrig, 1969; Habibagahi, 1973; Demars and Charles, 1982). Further temperature cycles yield comparatively minor, mostly reversible deformations as long as the maximal temperature of the first heat cycle is not exceeded. Thermal consolidation is a broadly measured phenomenon. Its effect is, however, more marked for reconstituted materials (Towhata and Kuntiwattanakul, 1994; Tanaka *et al.*, 1997) than for natural rocks.

The reduction of the strength of intact rock and the associated internal, irreversible deformation of the rock can lead to secondary consolidation effects. In case of a temperature decrease with its associated shrinkage of the intact rock and of the pore-water, suction will develop. This will lead to an adsorption of water without any significant non-elastic reverse deformations within the intact rock matrix.

33.2 Site-specific experimental information

Formation/site	Results and conclusions
Opalinus Clay in the Zürcher Weinland	Numerical modelling studies (Johnson *et al.*, 2001) and synoptic studies (Nagra, 2002). The consequences of the waste-derived heat pulse are very limited.
Boom Clay at Mol	*In situ tests:* CACTUS (Trentesaux 1997) and ATLAS (De Bruyn and Labat, 1998). *Laboratory tests:* Drained heating before submitting Boom Clay samples to triaxial CIU tests have been performed at two temperature levels (50 and 80°C). In both cases, the thermally-induced consolidation remains rather limited (de Bruyn 1999).
Boda Clay Formation at Mecsek	*In situ tests:* No irreversible thermally-induced consolidation effects were observed.

Of particular importance for the long-term development of a consolidation process is the change of permeability of the host rock. In thermal loading, permeability can principally be affected by two processes (Nagra, 2002):

(1) When considering the process of thermal consolidation as a deformation of a poro-elastic material, the relevant processes are the reduction of porosity and of permeability (Kozeny-Carman relationship; de Marsily, 1986). Beyond the irreversible changes due to first thermal loading, the net effects of a second thermal cycle (of comparable or lower intensity) on permeability remain negligible. For the formations considered, the first thermal loading occurred in the course of the geological burial.

(2) The second process of relevance is the possible formation, or reactivation, of discrete discontinuities or cracks due to additional thermal stress and increased pore-water pressure. A reduction of the effective stress (e.g. by an increase of the pore-water pressure) increases the over-consolidation ratio of the argillaceous material, resulting in dilatant deformation and fracturing (Horseman, 2001; see also FEP 42). Once the dilatant discontinuities are formed or reactivated, the permeability along them is increased, at least temporarily, by some orders of magnitude. This, in turn, assists in a subsequent reduction of the pore-water pressure and in associated reductions of the over-consolidation ratio, crack opening and permeability (Blümling *et al.*, 2001). Renewed mechanical loading and swelling then initiate a self-sealing process (Horseman, 2001) which will be further enhanced by the reduction of the pore-water pressure during or after the cooling phase. A precondition for fracturing to occur is that the effective stress level infringes the limiting strength conditions. At least in the case of the Opalinus Clay in the Zürcher Weinland, this is not the case (Nagra, 2002).

33.3 Scaling issues

With regard to the specification of the thermal pulse in space and time, no up- or downscaling is required. However, upscaling of the parameters describing the EDZ may be required (FEPs 37 and 40).

33.4 Scientific level of understanding

Current scientific understanding relies on combined knowledge of both the consolidation process proper and the effects of the relevant physical parameters. This knowledge is supported by a limited number of purpose-designed tests which have been carried out to date.

33.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 32	Thermal rock properties
FEP 37	Geomechanical rock properties
FEP 50	Past burial history

33.6 Level of understanding from a PA perspective and treatment in PA

This FEP is insensitive to PA models and generally not explicitly taken into account. It seems that the influence of this FEP remains limited.

33.7 Available reviews

None reported.

33.8 Planned work

None reported.

33.9 Overall evaluation

The understanding of this FEP relies on combined general knowledge of the consolidation process proper and on the effects of the physical parameters associated with the consolidation and heat dissipation processes in argillaceous materials. Only a very limited number of purpose-designed tests were carried out to date. Irrespectively of this, there is unanimous agreement that the influence of this FEP remains limited and it is seen as insensitive to PA models.

34. GEOMECHANICAL STABILITY (FEP B3.1)

34.1 Definition and generalities

In geotechnical engineering, the term *"stability"* is associated with the absence of large-scale failures or of excessive deformations which are detrimental to the function and safety of the engineered structure. In context with this FEP the term is associated mainly with the stability of the underground excavations of a repository and, to a minor degree, with the stability of boreholes in argillaceous rocks. The considerations on the stability of underground openings include the ground support system, if required. This FEP is a very important system component for the design and the operational phase of a repository. The geomechanical stability of the excavated underground openings is explicitly considered within the engineering analysis. Potential stability problems of the galleries after the emplacement of the waste and backfilling are considered to be irrelevant and are not addressed by this FEP. Furthermore, this FEP is neither associated with the global stability of the repository as a whole nor with the stability of geological host formation (e.g. the re-activation of a geological fault by increased pore-water pressures).

34.2 Site-specific experimental information

Formation/ site	Results and conclusions
Callovo-Oxfordian at Bure	*In situ at depths between 400 and 500 m:* Observation of borehole breakouts and ovalisation once the boreholes were passing through argillaceous layers.
Toarcian-Domerian at Tournemire	*In situ:* Monitoring during and after the excavation of two drifts, analysis of results and modelling of the mechanical response of the rock with time due to sequential excavation (Boisson, 2002).
Spanish Reference Clay in a Tertiary basin	The numerical code FLAC was employed in evaluating the effects of a tunnel on to the host rock in the following two formations: (1) In the Spanish Reference Clay (DM Iberia 1994) and (2) in the Opalinus Clay at Mont Terri (Velasco & Pedraza, 1997).
Boom Clay at Mol	Excavation of the Boom Clay at industrial scale has been demonstrated at a depth of 230 m. A convergence of about 9 cm (including about 4 cm of convergence ahead of the excavated front) is considered as acceptable for the long term performance of the repository. Excavation leads to fracturing of the clay body. Rigid lining is required to ensure the stability of the tunnel wall and to limit delayed convergence.

Formation/ site	**Results and conclusions**
Opalinus Clay at Mont Terri	*On-site information* from the New Gallery excavated in 1997-98: Bedding anisotropy has a major influence on stability: Bedding-parallel unloading fractures formed in the tunnel roof with some major breakouts. Sections without shotcrete lining are mostly stable if the tunnel is ventilated. Ventilation causes a drying out of the EDZ, thus increasing its strength. Major conclusion: Shotcrete lining in an Opalinus Clay repository might not be necessary, provided that the tunnel is ventilated with dry air and the bentonite backfill is installed in due time. In the tunnel excavation work, it is advisable to remove the high humidity at the excavation face by providing proper ventilation right up to the face. This increases the stability of the excavation and helps in preventing accidents. Swelling does not appear to be a problem for stability. At Mont Terri, the swelling capacity of the Opalinus Clay is quite limited (swelling pressures < 1 MPa; swelling heave < 10%). Long-term swelling heave was observed in the invert, but remained rather small. Boreholes show breakouts due to stress redistribution and bedding anisotropy. Generally, the observations made in the tunnels are also applicable to boreholes. *Regional evidence* in the Swiss Jura Mountains was collected by observations in railway and road tunnels in Opalinus Clay, some of them > 100 years old. Commonly, a massive concrete lining of the invert is installed.
Boda Clay Formation at Mecsek	*On-site experience* from tunnels in about 1 050 m depth: • The stability of the tunnels turned out to be significantly better in Boda Clay Formation than in sandstones, even in fractured zones. • Over the observation period of 5 years, there was no need for any remedial work in the Boda Clay Formation, even in the tectonised zones. • The only instabilities observed were local rock slabs and peels which developed immediately after excavation. No further instabilities occurred from about 2 weeks after the excavation. • There was a complete stabilisation of the convergence movements, even in tectonised zones. A possible exception is indications of ongoing movements in the invert (Martin 1994). • Boreholes in the Boda Clay Formation remained stable over > 15 years. *Numerical modelling:* Employment of UDEC and 3-D FEM codes (Dolexpert & ME-SCI 1998) supporting the on-site experience.
Mizunami Group at Tono	*In situ:* Long-term (several years) deformation monitoring was carried out after the excavation of a drift (JNC 1999b). The rate of displacement is < 0.5 mm in 3 years. Study on the scale effect of the mechanical properties: Several boreholes with different diameters (between 76 and 200 mm) in otherwise identical conditions. Rock failure tends to be more pronounced in bigger-diameter boreholes. *Numerical modelling:* 2D FEM studies on spacing of drifts and stability of the concrete lined underground openings at 500 m depth in soft rock (JNC, 1999b).

34.3 Scaling issues

Underground research laboratories and repository emplacement tunnels have similar dimensions, so no spatial upscaling is required. The observation time in underground research laboratories and tunnels extends over a time span of up to 100 years. The stability of the emplacement tunnels must be guaranteed over a time span of several years, so no upscaling in terms of time is required either. The same applies to other underground structures such as access tunnels, pilot and test facilities. Separate considerations might be necessary for underground storage tunnels for retrievable waste.

34.4 Scientific level of understanding

The level of understanding of this FEP is excellent. Reference can be made to a large body of knowledge from underground construction work in civil and mining engineering.

34.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 35	Size and structure of the EDZ
FEP 37	Geomechanical rock properties
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 38	Hydraulic properties of the EDZ
FEP 41	Swelling
FEP 42	Self-sealing
FEP 50	Past burial history
FEP 55	Present-day stress regime

34.6 Level of understanding from a PA perspective and treatment in PA

This FEP constitutes a very important system component for the design and for the early phase of a repository. It is critical for the functionality and safety of the technical operations. It is of no further concern after backfilling of the emplacement tunnel. Thus while it is important for the safety concept and for the operational phase, it is of no concern for PA. Generally, the level of understanding is considered to be sufficient (for short-term stability of up to some 10 years). However, this is not necessarily the case for the retrievability option, in which the geomechanical stability is of concern over a larger time scale.

The geomechanical stability of the excavated underground openings is explicitly considered within the engineering analysis of the repository. The methodology is in line with established engineering tunnel design procedures. The design includes the selection and dimensioning of the tunnel support system, if required.

34.7 Available reviews

Callovo-Oxfordian at Bure: AGEM (1998); Toarcian-Domerian at Tournemire: Boisson (2002).

34.8 Planned work

Formation/site	Planned activities
Callovo-Oxfordian at Bure	Vertical and horizontal mine-by tests with special emphasis on the influence of humidity on creep and rock strength. Predictive modelling of the mine-by tests; comparison of performance versus prediction; *a posteriori* modelling.
Toarcian-Domerian at Tournemire	Further laboratory mechanical tests; continuation of *in situ* measuring programmes; improvement of the rheological law for argillaceous rocks; modelling and validation.
Opalinus Clay at Mont Terri	Continuous modelling with numerical codes such as CODE_BRIGHT of some of the Mont Terri experiments; in the near future: EB and VE Experiments (Velasco & Pedraza, 1997).
Boom Clay at Mol	Fracturing around the excavation will be studied within the scope of the SELFRAC project.
Boda Clay Formation at Mecsek	Modelling programme with the existing field data.

34.9 Overall evaluation

This FEP is an important feature in the early phases of a repository. It is critical for the functionality and safety of the technical operations in the underground excavations throughout construction and operation. The level of understanding is excellent. Reference can be made to a large body of knowledge from underground construction work in civil and mining engineering. The studies required for PA are in line with established engineering tunnel design methods. The design includes the selection and dimensioning of the tunnel support system, if required.

In the case of a repository with the option for a retrieval of the waste, the long-term geomechanical stability of the underground excavations is less well understood and may need further attention.

35. SIZE AND STRUCTURE OF THE EDZ (FEP B3.2)

35.1 Definition and generalities

Underground excavation leads to a stress redistribution within the rock close to the excavated opening (tunnel, shaft, borehole). Depending on the excavation parameters (support type, excavation method and rate, size and shape of the opening, stress level, drilling fluid) and on the rock properties and their anisotropy, shear or tensile fractures (i.e. faults and joints) may develop in the adjacent rock. The EDZ (excavation-disturbed zone) includes not only the zone containing induced fractures (also termed "plastic zone") but also the distal part, which is characterised by elastic deformations due to excavation-induced stress changes (also termed "elastic zone").

Generally speaking, the more indurated the rock, the greater the likelihood of generating EDZ fractures. Over the long time period considered in PA, the counter effect (i.e. self-sealing, FEP 42) must be accounted for.

35.2 Site-specific experimental information

Formation/ site	Results and conclusions
Callovo-Oxfordian at Bure	Ovalisation and failure were observed in investigation boreholes penetrating the target formation. Based on numeric models for an unsupported gallery, the size of the EDZ was shown to extend from the excavated surface into the rock by about 75% of the excavation radius.
Toarcian-Domerian at Tournemire	Relevant information can be found in Boisson (2002) and Alheid *et al.* (1999). The underground research laboratory consists of a 110 years old tunnel (cross-section area 4.6 m x 5.7 m) and two galleries built in 1996, each 30 m long and with a circular cross-sectional area of 12 m^2. 500 days after the construction of the latter, convergence was max. 5 mm in the eastern, weakly fractured gallery. In the highly fractured and faulted western gallery, up to 23 mm were measured. Since then, convergence rates have decayed substantially. The EDZ of the 110 years old tunnel was cross cut and directly observed during the construction of the galleries. In the weakly fractured eastern wall, densely spaced vertical EDZ fractures (presumably joints) were identified up to 2 m away from the tunnel surface. In the western wall, the zone containing EDZ fractures is thinner, presumably due to the complexity of the pre-existing tectonic structures and their possible reactivation. Horizontal boreholes into the walls of the 110 years old tunnel yielded EDZ joints up to 1.35 m away from the tunnel surface, which corresponds to 0.27 times the average tunnel diameter. In the galleries from 1996, analogous boreholes yielded max. 0.6 m

Formation/ site	**Results and conclusions**
	thick zones containing EDZ joints (0.15 times the diameter of the galleries). Thus, related to the size of the underground opening, the EDZ is relatively smaller in the younger galleries when compared to the old tunnel. This is taken as evidence for the continued growth of the EDZ over decades after construction. Hydraulic conductivity of the EDZ was measured using the SEPPI probe and yielded enhanced values until 1.5 m in the case of the 110 years old tunnel and 0.6 m in the case of the galleries from 1996. Thus the hydraulic evidence is consistent with the structural observations. With some exceptions, no alteration rims along fractures can be observed. Gypsum and jarosite are found in some fractures.
Opalinus Clay at Mont Terri	Available evidence is summarised in Bossart *et al.* (2002) and Mazurek (2001). In boreholes drilled from the safety drift of the motorway tunnel, the EDZ can be subdivided into the following units as a function of distance from the wall of the drift: 0-70 cm: Inner part of the plastic zone, containing at least partly connected fracture networks. Small-scale transmissivity is in the order of 1 x 10^{-8} m^2/s. 70-200 cm: Outer part of the plastic zone with infrequent and mostly unconnected fractures. Transmissivity is much smaller (1 x 10^{-12} to 1 x 10^{-9} m^2/s). 200-400 cm: Elastic zone, defined by a slight increase of transmissivity when compared with the rocks in the far field of the tunnel. Macroscopic brittle fractures do not occur (data from ED-B Mine-by test, Martin & Lanyon 2002). In the framework of the Fracture Propagation experiment, 1 m long boreholes were drilled horizontally into the walls and vertically into the ceiling of the underground research laboratory. After impregnation with a fluorescent resin, these boreholes were overcored. The results are as follows (Bossart *et al.* 2002, Thury & Bossart 1999): • Extensional fractures along bedding planes were identified mainly in vertical boreholes penetrating the ceiling. • Extensional fractures in horizontal boreholes are near-vertical and parallel to the tunnel wall. They do not follow any pre-existing structures. • Tectonic shear fractures were identified in all boreholes, and about half of them were not impregnated, i.e. not reactivated and therefore tight. The frequency of extensional fractures is about 5 m^{-1}, in both horizontal and vertical boreholes. Reactivated shear fractures are more frequent in the ceiling (3 m^{-1}) than in the walls (1 m^{-1}), which possibly is an effect of gravitation. In a profile normal to the tunnel axis, the EDZ is dominated by concentric fractures. In a 3-D view, the fractures are tangential (i.e. parallel to the tunnel axis) in the walls, whereas they are parallel to bedding in the ceiling and thus have a dip angle of *ca.* 40° (with a dip direction parallel to the tunnel axis).

Formation/ site	Results and conclusions
Boom Clay at Mol	During the excavation of the Test Drift (end of 1987), there has not been a detailed characterisation of the size and structure of the EDZ. Only mapping of the fracture/discontinuity traces on the excavation walls was carried out. There is a debate on whether these planes are of tectonic origin and reactivated by the excavation, or if they are induced by the excavation. The recent excavation works (sinking of a shaft and starting chambers) showed evidence of fracturing around the new shaft, including fractures and slip surfaces showing a symmetry around the shaft axis (Barnichon & Bernier, 1999, Bernier *et al.*, 2000, Barnichon & Volckaert, 2003). The EDZ has been characterised during the excavation of the connecting gallery of the HADES underground research laboratory (fracture geometry, pore-water pressure and displacements). On the basis of model calculations assuming an elasto-plastic material law, the size of the plastic zone was estimated to be 5 m for a gallery with a diameter of 2.5 m (Bernier & Van Cauteren, 1999).
Mizunami Group at Tono	The EDZ was studied in the Tono mine before and after excavation of a new shaft and tunnel (Hirahara *et al.*, 1999, Sugihara *et al.*, 1998b). *In situ* measurements (displacements, and P-wave-velocity) indicate a size of the EDZ in the order of 1 m. P-wave velocity in the EDZ was about half that of intact rock. Finite-element model calculations of displacements and convergence due to excavation (Kamemura *et al.*, 1991) are consistent with *in situ* observations.
Boda Clay Formation at Mecsek	Due to the intense tectonic fracturing in the formation, the detection of fractures related to excavation is difficult. Indications exist from boreholes that the density of fractures parallel to the tunnel surface is slightly increased in the first tens of centimetres. Displacements and stress changes due to excavation were measured by various tools. These data were used in various geomechanical models predicting stress redistribution and related deformation. Model results were strongly affected by 1) bedding-related anisotropy and 2) a set of tunnel-parallel, steeply dipping fractures.

35.3 Scaling issues

The observations made in tunnels and shafts are at a relevant spatial scale for PA. However, there are some limitations regarding the evolution of the EDZ with time and on the connectivity of the EDZ fracture network on scales >1 m.

35.4 Scientific level of understanding

In indurated argillaceous rocks, both shear and extensional fractures and joints develop in consequence of excavation works. Even in soft clays (e.g. Boom Clay), fractures have been identified, even though with lower frequency and more limited hydraulic effects. The internal structure of the EDZ varies as a function of the material properties (incl. anisotropy), the orientation of the underground excavation and the orientation and magnitude of the regional stress regime. Geomechanical models predicting the size and structure of the EDZ are available and often provide results consistent with direct observations. In soft clays (e.g. Boom Clay), the characteristics of the EDZ are less well understood and require further data acquisition.

35.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 34	Geomechanical stability
FEP 37	Geomechanical rock properties
FEP 50	Past burial history
FEP 55	Present-day stress regime

35.6 Level of understanding from a PA perspective and treatment in PA

In general, the EDZ is represented in a simplified, conservative way for both soft and indurated formations. In some indurated formations, the EDZ is represented as a continuous higher-permeability zone. For Boom Clay, it is considered that the EDZ is a fractured domain. In PA, the effective thickness of the formation is considered to be 20 m smaller than its real thickness, thus accounting for a EDZ of 10 m (in radius) around each repository gallery.

35.7 Available reviews

NEA (2002b).

35.8 Planned work

Callovo-Oxfordian at Bure: The characterisation of the EDZ is a key subject of the planned experiments in the underground research laboratory at Bure. Additional tests will also be performed on the surface, especially regarding the influence of humidity on damage, failure and on rock strength. Predictive modelling of the planned two mine-by tests will be performed, focusing mainly on the size of the EDZ and its permeability. Later modelling stages (once experimental data are available) will mainly focus on the improvement of rheological models.

Boom Clay at Mol: The evolution of the EDZ with time will be studied in the frame of the SELFRAC project. This project includes modelling studies taking into account the delayed effects.

35.9 Overall evaluation

EDZ-related investigations are ongoing or are planned in several underground research laboratories. In spite of the growing knowledge, the EDZ is mostly treated in PA in a simplified, conservative way at the present stage. In many cases, it is assumed that no retention occurs in the EDZ, and the path length between repository and the exfiltration point of the host formation is reduced by the thickness of the EDZ. In order to reduce conservatism, more information is needed on the physical parameters of the EDZ and their evolution with time (e.g. self-sealing).

36. EFFECTS OF BENTONITE SWELLING ON THE HOST ROCK (FEP B3.3)

36.1 Definition and generalities

Bentonite-based backfill of waste emplacement tunnels is a fundamental component of the repository system in many designs. It can serve a variety of purposes, in particular: (1) Element of the multi-barrier system; (2) Element of the ground support system of the emplacement tunnel; (3) Element of imposing changes in the EDZ towards more favourable hydro-mechanical conditions, in particular towards lowering of the hydraulic conductivity, if possible to values which are intrinsic to the host rock (self-sealing; see also FEP 42).

With the water resaturation process of the EDZ after closure of an emplacement tunnel, water will seep into the emplacement tunnel, and the bentonite backfill will start swelling. At full saturation, the effects of swelling of the bentonite on the rock will, amongst others, depend on the composition and density of the backfill and on the convergence of the emplacement tunnel, i.e. the radial displacement of the EDZ towards the backfilled tunnel. If the density is comparatively low, swelling will predominantly be in form of *swelling strain* which will tend to close any existing voids. In confined conditions such as those of a fully backfilled and tightly packed emplacement tunnel, swelling will be predominantly manifested by *swelling pressures* which may rise to considerable magnitudes. These pressures will act as radial stresses onto the boundary (i.e. the excavation surface) of the emplacement tunnel. This effect causes increased confining pressures within the EDZ and tends to contribute to more stable conditions with regard to failure conditions and convergence movements, as long as the radial stresses do not exceed the tangential stresses at the excavation boundary. Increased confining pressures will change the material behaviour of the EDZ rock towards a more ductile behaviour. All these factors contribute to the effect of self-sealing of fractures within the EDZ.

Swelling strain and swelling pressure are interconnected parameters. The higher the swelling strain, the lower the swelling pressure, and *vice versa*. At equilibrium, the swelling stress of the bentonite backfill is of equal magnitude as the radial stresses at the excavation boundary, and the rates of the swelling strain and of the convergence become zero.

36.2 Site-specific experimental information

Formation/site/ reference	Investigation techniques employed	Results and conclusions
Spanish Reference Clay in a Tertiary basin (Enresa, 1999)	Numerical modelling	The effect of the bentonite swelling on the EDZ rock appears to be rather small for swelling pressures lower than 5 MPa.
Opalinus Clay at Mont Terri	SELFRAC *in situ* experiment	Bentonite swelling was simulated by load plates exerting pressure on the tunnel walls. A substantial decrease of transmissivity of EDZ fractures was observed. The experiment is currently ongoing.
Opalinus Clay in the Zürcher Weinland (Nagra, 2002)	Compilation of various types of investigations	At its placement the dry density of the bentonite backfill is 1.5 g/cm^3. The overburden height of 650 m is equivalent to a pressure of 15.6 MPa. Equilibrium between overburden and swelling pressures is established if the dry density of the bentonite is increased to 1.77 g/cm^3. This condition is reached by a volumetric compaction of the backfill of about 16% and a related convergence of the tunnel radius by max. 9%.
Boda Clay Formation at Mecsek	No purpose-designed investigations. Indirect observations from packer tests and their numerical modelling	Swelling of the backfill material can only marginally compensate the hydraulic deterioration of the EDZ.

36.3 Scaling issues

The analyses usually refer to limited time periods. Upscaling to PA time scales is required.

36.4 Scientific level of understanding

The swelling process of the bentonite in the backfill material is sufficiently well understood. This also applies to the effects of increased radial stresses at the inner boundary of the EDZ due to swelling and, generally, to the hydro-mechanical interaction between backfill and the EDZ. Problems exist in the understanding of the closure mechanisms of more complex fracture structures of the EDZ due to increased radial pressures. Such structures are, for example, arrays of interconnected extension and shear fractures and fracture plane wedges in the deeper parts of the EDZ.

36.5 Linked FEPs

FEP 33 Thermally induced consolidation of the host rock

FEP 35 Size and structure of the EDZ

FEP 37	Geomechanical rock properties
FEP 38	Hydraulic properties of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 55	Present-day stress regime

36.6 Level of understanding from a PA perspective and treatment in PA

The level of understanding is sufficient. So far, the process has been considered in PA in different ways. In the Spanish PA (Enresa, 1999), no consideration was made of the mechanical analysis of the emplacement system. The analysis was postponed for inclusion of further PAs in order to employ numerical codes which Enresa has been developing within its most recent R&D activities (e.g. CODE_BRIGHT). In the PA for Opalinus Clay in the Zürcher Weinland, the effects of bentonite swelling were explicitly considered.

Most conclusions are based on model calculations, and there are hardly any experimental results on the permeability changes which are caused by swelling strain and consolidation. In general, there is a need for site-specific information on the evolution of permeability of the EDZ after repository closure, i.e. of the various processes that contribute to self-sealing. This will necessitate extrapolation of experimental data from work undertaken in underground research laboratories. Such work is underway (see below).

36.7 Available reviews

None reported.

36.8 Planned work

Formation/site	Planned activities
Opalinus Clay at Mont Terri	*In situ* permeability tests of fracture planes under variation of the normal stress conditions. The changes are implemented from the tunnel excavation surface by means of a large-scale plate bearing test. This test is part of the EC SELFRAC project.
Boom Clay at Mol	Within the EC RESEAL shaft sealing test, the hydro-mechanical behaviour of the bentonite/Boom Clay interface is monitored and modelled.
Boda Clay Formation at Mecsek	Vague ideas on experiments in boreholes (e.g. sealing of boreholes and measurement of the hydraulic conductivity). Otherwise continuation and detailing of numerical modelling studies.

36.9 Overall evaluation

This FEP addresses a very important process in the affected field. The principal mechanisms associated with this FEP are regarded to be sufficiently well understood. This applies particularly to the swelling process of the bentonite and the hydro-mechanical interaction between the backfill and the EDZ rock. Problems exist in the understanding of the closure mechanisms of composite fracture structures of the EDZ under the effect of increased confining pressures. Examples of such composite structures are arrays of extensional and shear fractures and fracture plane wedges in the deeper parts of the EDZ.

37. GEOMECHANICAL ROCK PROPERTIES (FEP B3.4)

37.1 Definition and generalities

In a general sense, the term “geomechanical rock properties” relates to the mechanical characteristics of a rock. These characteristics include the generic mechanical behaviour (e.g. brittle or ductile) and the specific parameters that are commonly used to describe and specify the rock behaviour in mathematical terms.

In a narrow sense, the term is exclusively associated with the parameters which are used to specify the natural state of a rock (“state parameters”) and to determine its mechanical response to imposed loads and/or deformations in a model (“design parameters”; e.g. in a load test or a FE-model). Examples of “state parameters” are the density ρ, the water content w and the Atterberg Limits w_l and w_p. Examples of “design parameters” are Young’s modulus E, the strength parameters c and ϕ and the hydraulic conductivity K. The “design parameters” are intrinsically related to the material (“constitutive”) law chosen in the model.

Within this FEP, the term “geomechanical rock properties” is generally understood in the narrow sense.

Geomechanics is the science of the mechanical behaviour of soil and rock. Whilst argillaceous formations predominantly have rock-like features, they behave like soil in certain geological and technical conditions. This, for instance, is evidenced in the occasional usage of the Atterberg limits which constitute typical soil mechanical state parameters.

37.2 Site-specific experimental information

Formation/site	Results and conclusions
Callovo-Oxfordian at Bure	Results from laboratory experiments and numerical modelling (AGEM 1998, 1999): Determination of the deformability and strength parameters for three sub-units of the formation. Determination of some THM coupling parameters. Identification of a slight anisotropy of mechanical properties. Proposal of several constitutive laws for both short and long terms.
Toarcian-Domerian at Tournemire	Results from some laboratory and dilatometer tests (Barbreau & Boisson 1994, Niandou *et al.* 1997).
Spanish Reference Clay in a Tertiary basin	Data are documented in NEA (1999a).

Formation/site	Results and conclusions

Opalinus Clay at Mont Terri	The review by Bock (2000), considering 54 Technical Notes on laboratory, field and prototype tests in the underground research laboratory, resulted in a well constrained list of geomechanical parameters. Most design parameters sensitively depend on the water content w and the bedding anisotropy (⊥ normal to bedding; // parallel to bedding). Some of the more important parameters are as follows:
	Tangent modulus (50%): $E_{\perp}$ = 3 GPa; $E_{//}$ = 6 GPa
	Un- and re-loading modulus: $E_{\perp}$ = 6 GPa; $E_{//}$ = 12 GPa
	UCS (unconfined compressive strength) $UCS_{\perp}$ = 10 MPa; $UCS_{//}$ = 16 MPa
	UTS (unconfined tensile strength) $UTS_{\perp}$ = 1 MPa; $UCS_{//}$ = 2 MPa
	Shear strength of material: c’= 2.2 MPa; ϕ = 25°
	Shear strength of bedding planes: c’= 1.0 MPa; ϕ = 23°
	Dilatation of material $\Delta V/V_{\perp} = -2 \times 10^{-3}$; $\Delta V/V_{//} = -4 \times 10^{-3}$
	Dilatation angle i = 0°
	Swelling strain $S\varepsilon_{\perp}$ = 7%; $S\varepsilon_{//}$ = 1%
	Swelling pressure (at $S\varepsilon$ =0) $p_{s\perp}$ = 1.2 MPa; $p_{s//}$ = 0.6 MPa.

Boom Clay at Mol	Results from triaxial tests: Poisson ratio ν = 0.43, ϕ = 4°, c = 0.9 MPa, Young's modulus = 200-400 MPa, swelling pressure = 0.9 MPa, swelling strain = 0.5%. UCS = 2 MPa (CU-test), Plastic limit = 25%, Liquid limit = 55%, Plasticity index = 30%.
Yper Clay at Doel	Results from triaxial tests: ν = 0.23, ϕ = 10.2°, c = 0.4 MPa, Young's modulus = 50 MPa, swelling pressure = 1.2 MPa, swelling strain = 15%. UCS = 0.9 MPa (CU-test), Plastic limit = 30%, Liquid limit = 140%, Plasticity index = 110%.

Formation/site	Results and conclusions
Boda Clay Formation at Mecsek	*In situ tests* (sleeve fracturing; acoustic logging and empirical correlation with RMR methods, amongst them the Kiruna method; Hansagi 1978) yielded Young's moduli of 30-35 GPa in undisturbed and of 10 GPa in parts of tectonically disturbed zones. Ultrasonic tests yielded 40-60 GPa. Direct proof of a deformation anisotropy with $E_{//} \approx 2 * E_{\perp}$. Testing in the Delta-6 borehole indicated that the dynamic and static load responses are not very different: 46.4 GPa ± 25.4% (dynamic) versus 38.2 ± 40.4% (static from laboratory tests). A wide range of *uniaxial load laboratory tests* as part of the "Short-term Programme" (1995-1998) yielded, amongst others, data for Young's modulus E, Poisson's ratio ν, UCS, indirect UTS (Brazilian), wave velocity v_p and density ρ. Sub-sets of these parameters were evaluated as a function of (1) Geological position – (2) Tectonic structure (intact, crushed *etc.*) – (3) Petrology – (4) Direction of bedding anisotropy – (5) Size of the sample – (6) Overburden depth of the sample location. Cyclic load tests revealed a low degree of hysteresis. *Triaxial laboratory tests* on five different groups of samples. The geologically undisturbed samples revealed a cohesion of between 16 and 18 MPa and ϕ of about 37 to 41°. Against expectations, tectonised samples turned out not to have a substantially lower strength. Undrained triaxial tests were accomplished to delineate the influence of the pore-water pressure build-up. *Numerical experiments* of laboratory tests revealed that 2D UDEC and 3-D FEM numerical codes, with the provision for a linear elastic – ideally plastic behaviour and a Mohr-Coulomb strength criterion, are well applicable for the Boda Clay Formation. Prototype convergence measurements were recalculated by 2D-UDEC modelling and yielded the following revised material parameters: E = 40 GPa; $\nu = 0.20$; $\phi = 42°$; c = 17.5 MPa; UTS 6.5 MPa. The parameters of the Joint Set No. 1 are as follows (No. 2 in brackets, if different): $\phi = 42°$; c = 8,0 (17.5) MPa; UTS = 3 (6.5) MPa; $k_n = k_s$ (normal and shear stiffness) = 300 (30) Gpa/m.
Mizunami Group at Tono	Results are available from borehole jacking tests and seismic tomography (Sugihara *et al.*, 1998a, Matsui *et al.*, 1992) and from laboratory tests in connection with an EDZ *in situ* experiment carried out in the Tono mine.

37.3 Scaling issues

There is a general awareness of the need for upscaling of the laboratory test results (which apply to the cm to dm domain) and of the results obtained from underground research laboratories (which apply to the 1 to 10 metre domain) to the 100 to 1 000 m domain of the repository system. Upscaling of the parameters is common practice in rock mechanics. For the Boda Clay Formation and the Toarcian-Domerian at Tournemire, no satisfactory methods are available for such upscaling. For the Opalinus Clay at Mont Terri, evidence exists that, with regard to the deformational and strength parameters, the scale effect factor between the laboratory and repository dimensions is unusually low, i.e. close to unity (Bock, 2000):

- By common rock mechanics standards, the Opalinus Clay is a poorly fractured rock with an unusually high degree of homogeneity.
- One of its mechanically most important geological features are the bedding planes. They are pervasive structures and well represented even in comparatively small laboratory samples of the order of 10 to 100 millimetres. The results from the laboratory are therefore representative for a much larger scale.
- In Opalinus Clay, the shear strength parameters of discontinuities are not as drastically reduced in comparison to intact rock as is common in other types of rock (e.g. granite). In the review, it was shown that the effective cohesion c' and friction angle ϕ' of the material are not distinctively different from those of the bedding planes (and supposedly of the other joint planes). The dilatation angle i is close to zero.
- Successful numerical back analyses of the EDZ setting (size, geometry) in the Mont Terri underground research laboratory were carried out using laboratory-derived rock mechanical parameters. This is taken as evidence for the low relevance of the mechanical scaling factors.

37.4 Scientific level of understanding

When considering the common generic models that are routinely employed in soil and rock mechanics and in geotechnical engineering, the level of understanding seems to be sufficient with regard to the deformational, strength and permeability characteristics. The determination of the relevant parameters and the formulation of the underlying constitutive laws can be considered as standard procedures.

Deficiencies, however, exist in the fundamental understanding of the time-dependent creep processes of argillaceous rocks. The lack of understanding poses problems when extrapolating the test results to time scales that are relevant for PA. Conceptual, micro-mechanical models might assist to overcome such deficiencies. A micro-mechanical model, for instance, was developed for the Opalinus Clay (Bock 2001). It allows a substantially deeper insight into the relevant mechanisms than traditional generic models. In this model, material creep could be simulated by the PFC^{2D} computer code (trademark of the Itasca Comp.) as a continuous change of the structure of the clay platelets ("cataclastic flow") without relying on any traditional creep parameters.

37.5 Linked FEPs

FEP 14 Lithology, mineralogy of rocks and fracture infills

FEP 39 State of saturation of the EDZ and desiccation cracking

FEP 50 Past burial history

37.6 Level of understanding from a PA perspective and treatment in PA

The geomechanical properties of argillaceous rocks constitute fundamental data for any type of description, modelling and/or assessment of the mechanical behaviour of the formation in both far and affected fields and at any time. The specification of the geomechanical properties of the host rock is a basic pre-requisite for the disposal concept, for repository design and also some aspects of PA (e.g. migration of repository-derived gas, self-sealing, development of the EDZ). The properties have to be specified with regard to the deformational, strength, permeability and thermal behaviour of the rock.

The current level of understanding of the mechanical behaviour of the Callovo-Oxfordian at Bure is considered to be not sufficient for a quantitative treatment. Specifically, the coupling between desiccation and the mechanical properties needs more detailed investigations. In the PA of the Spanish Reference Clay, a mechanical analysis has still to be carried out (Enresa, 1999). There is the opinion that the rock mechanical data are adequately defined for use in the PA. For the Opalinus Clay, it is felt that the level of understanding reached is sufficient for repository design and PA. The relevant geomechanical effects are described and investigated by means of generic as well as micro-mechanical models.

For the Callovo-Oxfordian at Bure, the mechanical behaviour of the rock is described by a geomechanical conceptual model of the repository. The host rock is assumed to be a continuous porous medium and is subdivided into 3 units with regard to clay-mineral and carbonate content and mechanical characteristics. The constitutive laws have not yet been verified at the natural scale.

37.7 Available reviews

Formation/site	Document
Generic	NEA (1999a)
Callovo-Oxfordian at Bure	AGEM (1998, 1999)
Spanish Reference Clay in a Tertiary Basin	Enresa (1999)
Opalinus Clay in the Zürcher Weinland	Nagra (2002)

37.8 Planned work

Callovo-Oxfordian at Bure: Base-line information on the upscaling problem by carrying out of large-scale tests in the underground research laboratory to complement the existing data base from the laboratory tests.

Boom Clay at Mol: The short-term behaviour of the Boom Clay is now fully characterised. More effort will be devoted in the future to characterise the delayed effects (viscosity & pore-water dissipation).

37.9 Overall evaluation

The geomechanical properties of argillaceous rocks constitute fundamental data for any type of description, modelling and/or assessment of the mechanical behaviour of the formation in both the far and the affected field. The specification of the geomechanical properties of the host rock is a basic pre-requisite for the disposal concept, for repository design and also some aspects of PA (e.g. migration of repository-derived gas, self-sealing, development of the EDZ).

Deficiencies exist in the understanding of the time-dependent deformation processes (in generic terms: “creep”) of argillaceous materials. Conceptual micro-mechanical models provide a perspective to alleviate these deficiencies.

38. HYDRAULIC PROPERTIES OF THE EDZ (FEP B4.1)

38.1 Definition and generalities

The EDZ (see FEP 35) includes not only the zone containing induced fractures (also termed "plastic zone") but also the distal part, which is characterised by elastic deformations due to excavation-induced stress changes (also termed "elastic zone"). Both zones can have hydraulic properties that are different from those in the far field. These properties evolve with time in response to various processes that occur during the operational phase (e.g. stress redistribution, desiccation) and after backfilling (e.g. resaturation, swelling, self-sealing).

38.2 Site-specific experimental information

Formation/ site	**Type of information**	**Scale**	**Results and conclusions**
Toarcian-Domerian at Tournemire	*In situ* measurements from horizontal and sub-horizontal radial boreholes and on drillcores	cm – m	In the zone 0 to 1 or 2 m from the tunnel wall, hydraulic conductivity is 2 to 6 orders of magnitude larger than in the undisturbed rock (Alheid *et al.*, 1999, Boisson, 2002).
Opalinus Clay at Mont Terri	*In situ* measurements using different equipment and techniques (hydraulic, seismic and resistivity)	dm – m	Zone of about 1-2 m with increased hydraulic conductivity. Profile in the safety tunnel: • 0-0.7 m away from tunnel (inner part of the plastic zone): b T = 1 x 10^{-5} - 1 x 10^{-8} m^2/s; • 0.7 - 2 m (outer part of the plastic zone): T = 1 x 10^{-12} - 1 x 10^{-9} m^2/s; • 2-4 m (elastic zone): slightly enhanced transmissivities in spite of the absence of macroscopic fracturing (Martin & Lanyon 2002). All these measurements refer to a scale of dm and do not provide arguments regarding the larger-scale connectivity of EDZ fractures in either the radial or tangential direction. Crosshole responses and *in situ* resin impregnations in the first metre away from the tunnel indicate only limited tangential connectivity on a scale 0.5-1 m).

Formation/ site	**Type of information**	**Scale**	**Results and conclusions**
Boom Clay at Mol	*In situ* measurements in the underground research laboratory and samples taken around the "experimental shaft" of the underground research laboratory, back-analysis of the "Macro permeameter test"	cm – m	In the CP1 experiment, installed at the end of the part of the underground research laboratory that was constructed by using a freezing technique, the evolution of permeability was monitored over a few years. In this time period, the hydraulic conductivity dropped from 4 x 10^{-12} to 3 x 10^{-12} m/s at 8 m distance to the tunnel (this zone was strongly disturbed by freezing). Both of these values are very similar to the one referring to undisturbed rock. There appears to be no difference between hydraulic properties of the EDZ and undisturbed Boom Clay (Put, 2002). Laboratory measurements of hydraulic conductivity do not show any dependence on the distance to the tunnel surface (Volckaert *et al.*, 1995, Ortiz *et al.*, 1997).
Boda Clay Formation at Mecsek	*In situ* hydraulic tests and head measurements between 5 and 20 m from tunnel wall. 3-D hydro-mechanical modelling	m	Clear transient during blasting but no or very little influence on longer term beyond 5 m from tunnel wall. In the zone 0-5 m from the tunnel wall, the permeability is possibly enhanced by several orders of magnitude.
Mizunami Group at Tono	Measurements around shaft before and after excavation	m	Extent of influence (about 2 orders of magnitude) up to 1 m (Matsui, 1998).

Reliable techniques and equipment for the hydraulic characterisation of the EDZ are available. The zone of increased hydraulic conductivity is in general limited to one or a few metres around the galleries. The increase in hydraulic conductivity in the EDZ is substantial in indurated argillaceous formations (i.e. several orders of magnitude), and the contrast to the undisturbed zone is rather sharp. This increase in hydraulic conductivity can be attributed to fractures and interconnected fracture networks. In plastic clays, the hydraulic conductivity in the EDZ is similar to the one of undisturbed clay, at least around galleries or shafts that have already existed for several years. In this case the possible fracturing during excavation should seal relatively quickly. Similarly, even in indurated argillaceous formations, effects of self-sealing of the EDZ have been observed (FEP 42).

38.3 Scaling issues

As the radial extent of the EDZ is limited to a few metres, scaling in this direction is not an issue. However scaling of the hydraulic properties in longitudinal direction (e.g. degree of interconnection of fractures) or in time (e.g. self-sealing) remains an issue. Indications exist that the connectivity in the tangential direction is limited, leading to smaller hydraulic conductivities than measured on a small scale.

38.4 Scientific level of understanding

Although many observations and measurements are available, the scientific understanding of the development of the EDZ and the evolution of its hydraulic parameters with time is rather low.

38.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 6	Hydraulic properties of the host rock
FEP 33	Thermally induced consolidation of the host rock
FEP 34	Geomechanical stability
FEP 35	Size and structure of the EDZ
FEP 36	Effects of bentonite swelling on the host rock
FEP 37	Geomechanical rock properties
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 40	Coupled thermo-hydro-mechanic processes
FEP 41	Swelling
FEP 42	Self-sealing
FEP 55	Present-day stress regime

38.6 Level of understanding from a PA perspective and treatment in PA

For clays with high plasticity, there are strong indications that “self-sealing” will lead to a rather fast evolution of the hydraulic properties of the EDZ towards those of the undisturbed rock. In this case, from a PA point of view, there would be no difference in the hydraulic properties of the EDZ and the undisturbed rock.

For highly indurated argillaceous rocks, the understanding of the hydraulic properties of the EDZ, their evolution and the extent of the EDZ are more critical than in the case of plastic clays. In general, the understanding of the development of the EDZ during construction and its later evolution is rather limited. There are indications of self-sealing, but the process is slower and poorly understood. Due to these limitations, only a conservative treatment in PA is currently possible.

Mostly, this FEP is treated conservatively in PA, either by considering an effective thickness of the natural argillaceous barrier that is the real thickness minus the supposed thickness of the EDZ, or by considering a high permeability zone around the excavations. Often this is considered in combination with a “seal failure” or “poor sealing” scenario.

38.7 Available reviews

NEA(2002b).

38.8 Planned work

At Mont Terri, the EH project is continued to study the slow self-sealing process in the framework of the SELFRAC project. After resaturation of the EDZ, fracture transmissivity decreased substantially. Subsequently, bentonite swelling was simulated by load plates exerting pressure on the tunnel walls. Another substantial decrease of transmissivity of EDZ fractures was observed. The experiment is currently ongoing.

Both the EC CLIPEX and the SELFRAC projects study the effect of excavations on the development of the EDZ, its hydraulic properties and the potential for a subsequent self-sealing. In the underground research laboratory at Mol, the planned measurements (among others using the CLIPEX instrumentation) in relation to the excavation of the connection gallery should result in important information of the time evolution of the EDZ and the governing hydro-mechanical processes.

38.9 Overall evaluation

This FEP is of high importance because the evolution of the hydraulic properties of the EDZ determine to a large extent whether the EDZ can be a preferential pathway for radionuclide migration or whether it will behave similar to the undisturbed host rock. Currently there are many observations on the extent and evolution of the hydraulic properties of the EDZ, however the understanding of the hydro-mechanical processes governing the EDZ and its evolution is still rather poor.

39. STATE OF SATURATION OF EDZ AND DESICCATION CRACKING (FEP B4.2)

39.1 Definition and generalities

Ventilation of shafts and tunnels may result in desaturation of EDZ fractures or the rock matrix, especially where there is no lining or where a lining of the sliding rib type is used. This process potentially affects the geochemical, geomechanical and thermal properties of the EDZ.

Desiccation cracking is the result of shrinkage of an argillaceous material beyond the limits of a reversible material behaviour. Shrinkage is characterised by a *volume decrease* of the material. The physical reason for shrinkage is the lowering of the repulsion forces of the water bound to clay minerals (both “hydration water” and “double-layer water”) in connection with the evaporation of pore-water.

As with the underlying process of shrinkage, desiccation cracking is a *volumetric* feature. This means that cracking must be in the form of a (quasi homogeneous) fracture *pattern* and not in the form of discrete single structures. This characteristic constitutes a major difference to hydraulic and pneumatic fracturing (see FEP 47).

39.2 Site-specific experimental information

Formation/ site	Type of information	Results and conclusions
Toarcian-Domerian at Tournemire	Core drillings and direct observations of EDZ during chamber/gallery constructions	Unsaturated fractured zone of some tens of centimetres away from the tunnel surface (Boisson, 2002).
Opalinus Clay at Mont Terri	Core drillings and direct observations of EDZ during chamber/gallery constructions, TDR measurements, psychrometers, evaporation logging	High suction close to gallery wall, lower suction up to about 1 m depth. Suction indicates that the rock is not saturated, although the degree of desaturation can be quite low (Thury & Bossart, 1999). Thin gypsum coatings in fractures within the first 70 cm of rock adjacent to the tunnel surface indicate that 1) fractures in this zone are air-filled, and 2) a limited degree of evaporation of the matrix took place.

Formation/ site	Type of information	Results and conclusions
Boom Clay at Mol	Core drillings, *in situ* ventilation experiment (PHEBUS)	Unsaturated zone (but still with a high degree of saturation) behind permeable concrete lining of only about 20 cm, confirmation of small unsaturated zone by *in situ* ventilation experiment. No indication of dessication cracking (Robinet *et al.*, 1998).
Boda Clay Formation at Mecsek	Analysis of seepage water; *in situ* observations; no measurements of the degree of saturation of EDZ	Strong increase in salinity in pore-water attributed to evaporation by ventilation. *In situ:* Recognition of intense and widespread cracking of the formation in unlined tunnel walls. Besides desiccation due to the pre-cooled ventilation (~18 °C lower than the ambient temperature), various other reasons were identified for cracking: (1) Fracture system intrinsic to the rock; (2) Effects from stress redistribution (secondary stresses); (3) Effects from blasting. *In the laboratory:* Artificial desiccation cracking induced by maintaining a temperature of 80 °C over a time span of 2 months resulted in a considerable strength decrease of rock samples, with a reduction of the UCS of about 20 to 70%.

Several techniques are available to measure the degree of saturation of the unsaturated zone either by direct measurement on samples or by measuring the water potential (suction). In general the unsaturated zone around a gallery is limited to about 1 m or less and the degree of saturation remains rather high, except in macroscopic fractures, which may be completely dry.

The state of saturation has a strong influence on some geomechanical parameters, such as strength (Nagra, 2002, Daupley *et al.*, 1998). Desaturation leads to a hardening of the rock, which is beneficial for the geomechanical stability of the construction. Desication cracking is only observed is some argillaceous formations on galleries without lining.

39.3 Scaling issues

Experience exists on the laboratory sample and underground research laboratory scales and from geological evidence. No major problems exist in upscaling of the known features in terms of space and time to the repository scale.

39.4 Scientific level of understanding

The process of desaturation of the argillaceous formation by evaporation of water is well known and can be characterised by measuring the water retention curve (suction-water content relation) However, it is complicated by the presence of fractures in the EDZ that allow for an increased water exchange with the air in the gallery. The desaturation of the host rock, even when it is very small, can have a strong influence on other processes as oxidation, especially of pyrite, of the host rock and the increase of the salinity of the pore-water, both due to evaporation of water and oxidation. Thermal and geomechanical properties may also be affected, and these couplings are reasonably well studied.

It is generally felt that the mineralogical and physico-chemical reasons of desiccation cracking are sufficiently well understood. Deficiencies exist with regard to the *in situ* desiccation process caused by thermal loading.

39.5 Linked FEPs

FEP 32	Thermal rock properties
FEP 34	Geomechanical stability
FEP 35	Size and structure of the EDZ
FEP 37	Geomechanical rock properties
FEP 38	Hydraulic properties of the EDZ

39.6 Level of understanding from a PA perspective and treatment in PA

From a PA perspective, the state of saturation and its potential evolution with time is sufficiently well understood, however the understanding of the associated coupled processes is still too low to be accounted for in PA studies.

The importance of desiccation cracking for PA is considered to be rather minor, by consequence not much attention is given to this issue. Only a limited number of rather simple simulations were made to assess e.g. the time needed for resaturation. Within geomechanical modelling, desiccation cracking may be considered in an indirect manner, e.g. in the form of a generic increase of the strength or permeability parameters. It is not considered to be a component of the repository system that would require explicit formulation.

39.7 Available reviews

None reported.

39.8 Planned work

Both at Mol and Mont Terri, further experiments are foreseen either in the framework of EDZ studies or investigations of the influence of ventilation on the disturbed zone. The VE experiment at Mont Terri investigates the state of saturation of the EDZ 1) at the time of the excavation of a new tunnel and 2) 1 year later. Results are expected in 2003-2004.

39.9 Overall evaluation

As the extent of the unsaturated zone is small, the importance of this FEP is from a hydraulic point of view rather low. However, this FEP can have a strong influence on the pore-water chemistry in the EDZ, especially at sites where the EDZ fracture system would remain open and interconnected for a long time.

Desiccation cracking is a geomechanical phenomenon which is sufficiently well understood. It might occur locally within the backfill material and/or in the EDZ. In geomechanical modelling, desiccation cracks are not specifically modelled but may be considered in an indirect manner, e.g. by an adjustment of the strength or permeability parameters.

40. COUPLED THERMO-HYDRO-MECHANIC PROCESSES (FEP B5.1)

40.1 Definition and generalities

The generation of heat that will dissipate into the backfill and the surrounding host rock is a well-known characteristic of high-level radioactive waste emplaced in the underground. The associated mechanical, hydraulic, thermal and chemical effects are of potential importance for the behaviour of the repository system, particularly in the affected field. In the far field, the effects are limited as long as possible pore-water pressure and effective stress variations remain within acceptable limits.

High-level radioactive waste constitutes a decaying heat source. For the surrounding host rock, this implies that, after the heating stage, which is initiated at the time of waste emplacement, there will also be a cooling phase with a convergence towards the re-establishment of the natural thermal conditions. The time span over which such a heat pulse is acting depends on the type of waste (less important for vitrified high-level waste and more important for spent fuel). Commonly it is of the order of some 1 000 to some 10 000 y. The thermal impact is negligible for all other types of waste.

The heat pulse causes complex mechanical, hydraulic and chemical interactions in the host rock, and all phases (gas, liquid, solid) need to be considered. Coupled thermal-hydraulic-mechanical (THM) models are generally required to adequately describe the repository response to the heat pulse. Of particular importance are thermally triggered changes in the transport of the fluids (hydraulic conductivity, gradient) and a possible non-linear behaviour of the solids, e.g. in form of permanent deformations due to consolidation or due to cracking and fracturing (“heat cracks”; deterioration of the rock material under the influence of heat). The influence of heat on hydraulic conductivity is well known and is due to the decrease of viscosity of water with increasing temperature.

40.2 Site-specific experimental information

Formation/site	Results and conclusions
Opalinus Clay in the Zürcher Weinland	Numerical modelling studies (Johnson *et al.*, 2001, Nagra, 2002).
Boom Clay at Mol	Coupled THM experiments (ATLAS, CACTUS, CERBERUS), numerical modeling of ATLAS in INTERCLAY 2.

In the PA for Opalinus Clay in the Zürcher Weinland, the main results are as follows: The maximum temperature that can be expected to occur at the contact between the bentonite backfill and the Opalinus Clay (EDZ) is 95°C. According to the very conservative model computations, temperatures in excess of 80°C are reached about 10 years after the emplacement of the waste. The maximum temperature of 95°C is reached some 100 years after emplacement and is reduced to about

80°C after about 1 000 years. The Opalinus Clay is thus subjected to a temperature that is slightly higher than the maximum temperature of its geological past (*ca.* 85°C). The excess temperature of 10°C is effective in the direct vicinity of the emplacement tunnels and is prevailing over a (geologically) rather short time span. In the first 1 000 years after the emplacement, both the bentonite backfill and the rock in the EDZ are only partially saturated. The resulting high suction pressures and the existence of a hydraulic gradient will cause a water transport from the surrounding host rock towards the emplacement tunnels. The quantitative analysis of coupled effects associated to the thermal pulse yielded the following main results (Nagra, 2002, ch. 7.6.3):

- The most relevant effect is the increase of pore pressure (by max. 7 MPa at the interface of bentonite backfill and host rock, if the drainage that developed during construction and operation is conservatively neglected). However, no fracturing is expected in connection to this effect.

- Chemical, hydraulic and mechanical effects (see also FEPs 31 and 33) are of minor importance.

For plastic clays with high water content, a qualitatively similar behaviour has been observed in the framework of the ATLAS, CACTUS and CERBERUS *in situ* THM experiments in Boom Clay at Mol. During heating, the thermal expansion of water induces a fast increase of pore-water pressure and total stress. Following the thermal pulse, pore-water pressure dissipates more quickly than total stress, resulting in a consolidation of the clay. These experiments show a qualitative similarity between the behaviour of clay submitted to a thermal load and to a total stress increase.

40.3 Scaling issues

With regard to the understanding of the thermal pulse in space and time, no up- or downscaling is required. Upscaling might, however, be required for the mechanical and hydraulic properties (see FEPs 37 and 38).

40.4 Scientific level of understanding

The scientific level of understanding of this FEP is quite advanced. The following table summarises the possible hydro-mechanical effects of a heat pulse.

Process	Possible consequences
Thermal expansion of the material (bentonite and rock) and of the pore-water	Pore pressure increase Change of effective stress Strength reduction of the material Lowering of threshold value for the onset of creep Increase of creep rate
Thermally-induced consolidation (treated in FEP 33)	Additional flow of water Decrease of porosity and permeability

Thermal expansion: A temperature change influences the strength of a saturated material such as bentonite or rock by means of changes of the pore-water pressure and thus of the state of effective stress. According to Campanella & Mitchell (1968) and Horseman (1994), the change of the pore-water pressure in an argillaceous material due to a temperature increase can be specified as follows:

$\Delta p = F * \Delta T * \sigma'$ with:
Δp = change of pore-water pressure
ΔT = temperature change
σ' = effective stress
F = Mitchell factor.

The Mitchell factor F is specified as follows:

$F = e_0 ((\alpha_s - \alpha_w) + \alpha_{st}/n)/0.434\ C_s$, where
e_0 = initial void ratio
n = porosity
α_s = coefficient of thermal expansion of the intact rock
α_w = coefficient of thermal expansion of water
α_{st} = physico-chemical coefficient of expansion
C_s = swelling coefficient.

This equation shows that the Mitchell factor F is essentially controlled by three parameters:

1. The thermal expansion coefficient of water. The coefficient of thermal expansion of the rock matrix is of less significance as it is typically one order of magnitude smaller than that of water.
2. The physico-chemical coefficient of expansion of the texture of the argillaceous material α_{st}. This coefficient is different from that of the thermal expansion of the clay-mineral platelets as it is significantly affected by the changes of the adhesive forces of water and of the osmotic forces. According to Campanella & Mitchell (1968) the parameter α_{st} is about $-0.5*10^{-4}$ °C^{-1}.
3. The swelling coefficient C_s, which describes the compressibility of the rock matrix. C_s can best be deduced from the so-called storage coefficient (Horseman 2002). From hydraulic tests the storage coefficient of the Opalinus Clay was determined at $1.5 \times 10^{-5}\ m^{-1}$.

The level of scientific understanding of further thermally-induced expansion effects (see Table above) is discussed in Nagra (2002, ch. 7.6). The effects include the strength reduction of the material, the lowering of threshold value for the onset of creep and the increase of creep rate. Calculations show that all these effects are not relevant at least in the case of Opalinus Clay.

Thermal consolidation and secondary compaction: According to Campanella & Mitchell (1968), subjecting an argillaceous material to a temperature increase leads to a consolidation process which is similar to conventional mechanical consolidation (thermal stress instead of mechanical stress; see FEP 33).

40.5 Linked FEPs

FEP 32	Thermal rock properties
FEP 33	Thermally induced consolidation of the host rock
FEP 35	Size and structure of the EDZ
FEP 37	Geomechanical rock properties
FEP 38	Hydraulic properties of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking

40.6 Level of understanding from a PA perspective and treatment in PA

The level of understanding appears sufficient for a PA. The most significant disturbance caused by a heat pulse is the transient increase of the pore-water pressure in most parts of the geological repository. The excess pore-water pressure, however, is released (1) by squeezing out of pore-water and (2) by subsequent lowering of the temperature due to the decay of the heat pulse.

For a PA this FEP has to be covered by extensive numerical modelling studies. The studies have to be based on highly specialised T-H-M coupled numerical codes. Appropriate codes are commercially available from various sources. However, there still seems to be a lack of reliable site-specific parameter sets and of reference sites for the validation of coupled T-H-M numerical models.

40.7 Available reviews

None reported.

40.8 Planned work

Formation/site	Planned activities
Opalinus Clay at Mont Terri	The HE-heater experiment, including modelling of thermally induced H-M effects.
Boom Clay at Mol	Large heater experiment and associated numerical modelling.

40.9 Overall evaluation

The level of generic understanding of this FEP is quite advanced. The thermal expansion of a saturated rock is predominantly controlled by the coefficient of thermal expansion of the water. The respective coefficient of the rock matrix is of less significance as it is typically by about one order of magnitude smaller than that of water. A temperature change influences the strength of a saturated material predominantly by means of changes of the pore-water pressure and thus of the state of effective stress.

The most significant disturbance caused by a HLW heat pulse is the transient increase of the pore-water pressure in most parts of the geological repository. The excess pore-water pressure, however, is released (1) by squeezing out of pore-water and (2) by subsequent lowering of the temperature due to the decay of the heat pulse.

41. SWELLING (FEP B5.2, C2.3)

41.1 Definition and generalities

Swelling is a volume increase of a material (argillaceous host rock in the EDZ or backfill in the emplacement gallery) due to adsorption of water on clay minerals. Nüesch (1991) distinguishes “inner-crystalline swelling” due to the insertion of hydration water and “osmotic swelling” due to the adsorption of diffuse double-layer water. In confined conditions, as is typical for both a tightly backfilled emplacement gallery and the EDZ, swelling pressures of considerable magnitude can develop.

Swelling is one of the processes that contribute to self-sealing of the EDZ as well as of natural fractures (see FEP 42). The capacity of an argillaceous rock to swell when exposed to free water depends on: (a) clay mineralogy, (b) degree of cementation of the matrix, (c) stress history, and (d) water chemistry. Water is drawn into the clay fabric by physico-chemical forces, and this inward movement of water molecules into the interparticle spaces causes the fabric to expand. In unconfined conditions the resulting volumetric strain is always substantially larger than what can be explained by invoking simple poroelastic concepts. The presence of an interparticle cement can inhibit swelling of the clay fabric. However, cementing agents such as calcite and silica tend to behave in a brittle manner and are easily damaged in the formation process of the EDZ. In fact, it appears likely that fabric damage is a necessary pre-requisite for swelling in some argillaceous rocks. Many argillaceous rocks also exhibit a progressive process of fabric breakdown referred to as softening. This is a gradual alteration of a hard rock into a plastic soil-like clay material with substantially reduced shear strength (Bott 1986). The water content of a softened argillaceous rock is significantly larger than that of the parent material showing that swelling and softening are closely interlinked. Softening commences around fissures and fractures. It seems likely that the combined processes of swelling and softening will lead to a gradual decrease of fracture permeability.

41.2 Site-specific experimental information

Formation/site	Investigation techniques employed	Results and conclusions
Toarcian-Domerian at Tournemire	Laboratory swelling and shrinkage tests on samples from boreholes (equiv. oedometer cells with *in situ* water)	Swelling pressure normal and parallel to bedding: $p_{s \perp ss}$ = 0.1 to 0.6 MPa $p_{s // ss}$ = 0.3 to 0.5 MPa. Swelling strain anisotropy (normal/parallel): 0.4-1.3. Swelling strain normal to bedding: 1.3-1.5%. Rather low swelling pressure under natural confining pressure. Shrinkage-swelling cycles show a hysteresis, probably linked to changes in the texture of the material (Daupley, 1997, Boisson *et al.*, 1998).
Callovo-Oxfordian at Bure	Laboratory swelling and shrinkage/swelling tests (oedometer and triaxial) Numerical modelling on the effects of ventilation on the host rock	Swelling pressure of about 0.8 to 1 MPa (in oedometer tests). Swelling occurs even under 12 MPa confining pressure (in triaxial tests; Andra, 1998). Part of shrinkage is irreversible (in cyclic shrinkage-swelling tests; Andra, 1999b).
Opalinus Clay at Mont Terri (Bock 2000)	Laboratory experiments	Swelling pressure normal and parallel to bedding: $p_{s \perp ss}$ = 1.2 MPa $p_{s // ss}$ = 0.6 MPa.
Boom Clay at Mol (Ortiz *et al.* 1997)	Laboratory analysis: presence of swelling clay minerals	Swelling pressure ≈ 1 MPa, measurement of permeability as a function of swelling shows maximum increase by less then a factor 2.

41.3 Scaling issues

Beyond the laboratory scale as described above, this FEP can, in principle, be characterised at full scale in underground research laboratories. Experiments will be limited to practical time periods (a few years maximum) and it is necessary to make extrapolations of the behaviour over much longer PA time scales.

41.4 Scientific level of understanding

Generally, the level of understanding of swelling and of the underlying physico-chemical processes is reasonably good.

41.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture water composition
FEP 30	Organics from waste and their effect on transport properties of the host rock
FEP 37	Geomechanical rock properties
FEP 38	Hydraulic properties of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)

41.6 Level of understanding from a PA perspective and treatment in PA

The level of generic understanding of swelling is generally quite good. It needs to be considered in several aspects of site characterisation, repository design and PA:

- Numerous case studies in civil and mining underground construction have demonstrated the particular importance of swelling for the design and excavation of the repository tunnels and galleries and of the ground support system.

- Swelling is one of the major causes of borehole instability in argillaceous formations. Purpose-designed drilling fluids or dry drilling can minimise the effects. It also has (often undesired) effects on *in situ* tests and experiments (e.g. hydraulic and geomechanical characterisation).

- Laboratory experiments (e.g. percolation and diffusion tests) may be affected by swelling. In many cases, swelling and related self-sealing are welcome effects because they reduce the likelihood of artificial short-circuits. On the other hand, the volume change related to water saturation under unconfined laboratory conditions may be an undesired effect. At least for Opalinus Clay, it was shown that saturation under unconfined conditions results in water contents well above those that refer to *in situ* conditions, with consequences for the parameters that are characterised by the experiment (e.g. shear strength).

- Swelling is one of the mechanisms underlying self-sealing and thus plays a role for the development of the hydraulic characteristics of the EDZ as well as of natural fractures.

In spite of a generally good generic understanding, site-specific characterisation and parametrisation at appropriate scales is less well developed. Insufficient experimental results are available from on-site tests and observations. In general, there is a definite need for site-specific information on the permeability of the EDZ over the time period of PA. This will necessitate extrapolation of experimental data from work undertaken in underground research laboratories. Such information would also be useful for the understanding of self-sealing in natural fractures.

41.7 Available reviews

None reported.

41.8 Planned work

None reported.

41.9 Overall evaluation

This FEP is important for site characterisation, construction and PA. It needs to be explicitly considered in the design of the underground structures of the repository. It has major repercussions on the time-dependent development of the permeability characteristics of the EDZ and is one of the keys in triggering self-sealing of repository-induced fractures. The capacity of swelling and, implicitly, of self-sealing needs to be examined on a rock- and site-specific basis.

42. SELF-SEALING (FEP B5.3, C2.4)

42.1 Definition and generalities

Self-sealing is a process that leads to a reduction to the hydraulic transmissivity of a fracture. On the other hand, *self-healing* includes the reduction in the impact of a fracture on both the hydraulic and mechanical properties of the rock mass (Horseman, 2001).

The capacity of fractures in argillaceous rocks to self-seal (or become, with the passage of time, less conductive to ground water) is often cited as a primary factor favouring the choice of such materials as host rocks for deep disposal. Self-sealing mechanisms have been widely observed in a variety of argillaceous rocks. The underlying processes which contribute to self-sealing can be broadly subdivided into two categories: (a) hydro-mechanical processes linked to the change in the stress field, the movement of water and time-dependent rock deformation, and (b) geochemical processes linked to changes in both the composition and the fabric of the rock.

Horseman (2001) emphasised the role of hydro-mechanical processes in self-sealing and suggested that the main consideration in assessing the capacity for self-sealing is the temporal evolution of the stress path. Qualitative arguments were based on the Modified Cam-Clay Model which describes the deformation and failure of porous rocks. The state boundary surface is assumed to comprise the Hvorslev Surface for material on the “dry side” of the critical state line and the Roscoe Surface for material on the "wet side" (Shah, 1997). Shear deformation on the “dry side” favours dilatant shear fracturing, whereas shear deformation on the “wet side” favours contractant behaviour. According to this model, the EDZ is formed when the stress path touches the Hvorslev surface. The combined effect of stress relief and shear-induced dilatancy is a significant reduction in the pore-water pressure. It seems probable that pore-water pressures can actually become negative in sign (i.e. a state of suction) close to the walls of the repository excavation, leading to localised de-saturation. The dilatant response will also lead to a measurable increase in the permeability of the EDZ.

Within this FEP, the self-sealing of migration pathways is considered, irrespectively of whether these pathways are natural or man-induced in origin. Self-sealing may occur in natural fractures subsequent to movements along these (e.g. due to earthquakes, fault (re)activation, uplift and subsidence) or in EDZ fractures (e.g. due to resaturation, swelling pressures of bentonite-based backfills, creep). Self-sealing in argillaceous rocks can be triggered essentially by three mechanisms:

1. Closing of fractures (pathways) by swelling, i.e. a volume increase of some clay minerals (mainly of the smectite group) by water uptake (see FEP 41);
2. Filling of fissures and fractures through the generation of infilling materials or mineral precipitation;
3. Closing of fractures (pathways) resulting from mechanical deformation, i.e. plastic deformation of the argillaceous layer under the acting geomechanical stress field.

In many cases these mechanisms will occur simultaneously and will complement each other.

42.2 Site-specific experimental information

Formation/site/ reference	Investigation techniques employed	Results and conclusions
Opalinus Clay at Mont Terri (Einstein *et al.*, 1995; Meier *et al.*, 2000; Enachescu *et al.*, 2002)	EH/SELFRAC Experiment at Mont Terri: *In situ* measurement of the change of the transmissivity of an artificially-induced crack in consequence of resaturation and by increase of the effective normal pressure by > 2 MPa	Decrease of transmissivity from ~ 2 x 10^{-8} m^2/s (for open cracks) to ~ 5 x 10^{-13} m^2/s (which is almost identical to the undisturbed rock).
Adler *et al.*, (2001)	Laboratory percolation tests	A drillcore with an artificially induced fracture across the entire core length was installed in an infiltration apparatus at 60 bar confining pressure (close to *in situ* lithostatic conditions at Mont Terri). A fluid pressure difference of 30 bar across the core resulted in forced advection. From the beginning on, hydraulic conductivity was similar to the one of the undisturbed matrix. Flow occurred throughout the core, with no preference towards the fracture. The first water sample was taken a few days after starting the experiment, and its composition was characteristic of *in situ* pore-water, with no traces of the chemically different fluid that was infiltrated at the upstream side. Thus complete self-sealing of the fracture occurred very quickly.
Opalinus Clay in tunnels of the Swiss Jura Mountains (Gautschi, 2001)	*In situ* observations in existing railway tunnels	No water seepages identified at overburden heights > 200 m (in total 6 600 tunnel metres in Opalinus Clay).
Boom Clay at Mol (Ortiz *et al.* 1997)	*In situ:* A hydraulic frac test was carried out in a horizontal borehole four months after a gas injection test (see also FEP 47).	The measured hydraulic conductivity was identical to that of the undisturbed clay (1.57 x 10^{-12} m/s), indicative of rapid self-sealing.
	Mine-by test: measurement of hydraulic reactions around excavations	Hydraulic pressure profile shows fast sealing of excavation-induced fractures. Swelling and plasticity are expected to seal fractures.

Formation/site/ reference	Investigation techniques employed	Results and conclusions
Boda Clay Formation at Mecsek	*In situ:* Non-systematic observations in the underground research laboratory and in surface boreholes of fracture zones and mineral infillings. Hydraulic tests.	Softening of water-conducting fracture surfaces with a reduction of flow to zero and softening of borehole walls in sleeve fracturing tests with a reduction of E from ~30 GPa to < 2 GPa over a time span of ~3 years. The water inflow into a nearly 600 m long borehole section decreased from about 1.0 l/min to < 0.2 l/min over a time span of 10 years.

42.3 Scaling issues

The rates at which self-sealing occurs in indurated formations in the EDZ of an emplacement tunnel or in natural fractures is difficult to assess at the present stage. Long-term experiments in underground research laboratories could provide additional constraints.

The degree to which fracture mineralisations that occurred in the past ("palaeo-self-sealing") can be used as arguments to constrain future behaviour needs to be established carefully, i.e. the physico-chemical conditions at which mineralisation took place must be shown to be comparable to the present-day situation.

42.4 Scientific level of understanding

The basic physico-chemical and hydro-mechanical processes leading to self-sealing are rather well understood. In principle, models and many data are available to enable a reasonable understanding of many aspects of self-sealing. However, the modelling of the overall self-sealing process, especially when several processes occur simultaneously, remains a very difficult task. Often the knowledge of the geological history of the formation of a migration pathway is insufficient to allow a detailed modelling of geological self-sealing processes.

One of the main uncertainties is associated with the currently limited capability to predict the effects of self-sealing on advective transport in the EDZ or in a natural fracture over the time period which is relevant for PA. The role of self-sealing is likely to be rock-specific.

42.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 17	Pore- and fracture water composition
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 29	Interactions of hyperalkaline fluids and host rock
FEP 36	Effects of bentonite swelling on the host rock
FEP 37	Geomechanical rock properties

FEP 38	Hydraulic properties of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 41	Swelling
FEP 50	Past burial history
FEP 52	Future changes in hydrochemistry of the host rock and of surrounding formations (e.g. due to out-diffusion, water-rock interactions, uplift)
FEP 56	Future stress regime

42.6 Level of understanding from a PA perspective and treatment in PA

This FEP is used in PA studies mostly at the scenario development stage. From a PA perspective, the current level of understanding of self-sealing mechanisms is sufficient to judge whether in a given argillaceous formation newly formed fractures could remain open, i.e. remain important migration pathways for a long time or not. However, the detailed modelling of the closure of such migration pathways, especially by infilling minerals, remains difficult. There are few examples (e.g. the Opalinus Clay PA) of the assessment of the possible effect of fractures on the overall safety of a repository.

42.7 Available reviews

The current level of understanding is summarised in Horseman (2001). The NEA has commissioned an overview report on the self-sealing of fractures under repository conditions.

42.8 Planned work

In the EC project SELFRAC, the self-sealing mechanisms in Boom Clay and Opalinus Clay are studied, at Mont Terri the EH self-sealing test is still ongoing. Although these projects are mainly oriented on self-sealing of the EDZ, they will increase our understanding of self-sealing processes in general.

Formation/site	Planned activities
Generic/several sites	A synthetic overview of the underlying processes and compilation of empiric evidence for self-sealing is currently being elaborated at the British Geological Survey. This project was commissioned by the Clay Club, a working group of the NEA.
Callovo-Oxfordian at Bure	Self-sealing studies are in progress within the framework of the Andra-sponsored FORPRO French research network.
Opalinus Clay at Mont Terri	*In situ* permeability tests of fracture planes under variation of the normal stress conditions. The changes are implemented from the tunnel excavation surface by means of a large-scale plate bearing test. This test is part of the SELFRAC project.
Boom Clay at Mol	Self-sealing studies are in progress within the framework of the EU project SELFRAC.

42.9 Overall evaluation

For disposal in argillaceous formations, this FEP is very important as self-sealing of migration pathways is a process that can give a very large contribution to the confining properties of argillaceous host rocks and to the robustness of disposal in argillaceous materials. Self-sealing is expected to occur in a wide variety of argillaceous formations. Although the understanding of self-sealing processes is already well-developed, studies should be continued to allow more quantitative assessments.

43. OFF-DIAGONAL ONSAGER PROCESSES EXCEPT CHEMICAL OSMOSIS (FEP B5.4)

43.1 Definition and generalities

In the framework of the theory of irreversible thermodynamics, a given flux J_i (e.g. a flux of heat, fluid, solutes or electrical charge) can be expressed as

$$J_i = \Sigma_j L_{ij} X_j$$

where the X_j terms are driving forces (e.g. temperature, hydraulic, concentration, or electrical potential gradients), and the L_{ij} terms are the so-called phenomenological coefficients. The term direct or diagonal phenomena is used for the ($L_{ii} X_i$) contribution to a flux J_i, and the term coupled or off-diagonal phenomena is used for a ($L_{ij} X_j$) contribution ($j \neq i$). The phenomenological coefficients are related by the Onsager Reciprocal Relation: $L_{ij} = L_{ji}$. The following table is a matrix of direct (diagonal) and coupled (off-diagonal) transport phenomena.

	POTENTIAL GRADIENT X			
FLUX J	**Temperature**	**Hydraulic**	**Chemical**	**Electrical**
Heat	Thermal conduction Fourier's Law	Thermal filtration (Isothermal heat transfer)	Dufour effect	Peltier effect
Fluid	Thermal osmosis	Advection Darcy's Law	Chemical osmosis	Electrical osmosis
Solute	Soret effect (Thermal diffusion)	Hyperfiltration	Diffusion Fick's Law	Electrophoresis
Current	Seebeck or Thompson effect (Streaming current)	Rouss effect	Diffusion and Membrane potentials	Electrical conduction Ohm's law

Off-diagonal processes can occur in any type of host rock, but are likely to be most pronounced in unfractured rock of high clay-mineral content. Their primary relevance is to the affected field where the maximum driving forces (gradients) are present. Two off-diagonal processes, chemical osmosis and hyperfiltration, have been examined in detail in several site studies because of their possible influence on site properties and their characterisation.

This FEP discusses scoping calculations on the relative importance to repository performance of all coupled phenomena except those including electric potentials or currents, which are not considered relevant. The focus is on processes in the affected field. Chemical osmosis is a mechanism that may have some relevance for the characterisation of the far field, and these aspects are discussed in FEP 44.

43.2 Site-specific experimental information

The importance of off-diagonal processes has been evaluated in field and laboratory studies and theoretically, using site-specific, literature and bounding values for coupling coefficients. Studies relevant to waste management are summarised in the following table:

Formation/site	Type of Study	Coupling(s) Investigated	References
Callovo-Oxfordian at Bure	Field / scoping calculation	Chemical osmosis	Andra (1999a)
Opalinus Clay at Mont Terri under representative repository conditions	Theoretical	All except electrical	Soler (1999, 2001)
Opalinus Clay at Mont Terri	Field and laboratory	Chemical osmosis	Harrington & Horseman (1999, 2000); continuing work in progress; see FEP 44
Boom Clay at Mol	Laboratory	Hyperfiltration	in progress
Pierre Shale in south Dakota	Field	Chemical osmosis	Neuzil (1994, 2000); See FEP 44
Kaolinite and Wyoming Bentonite under assumed repository conditions	Theoretical	All except electrical	Carnahan (1984, 1985) summarised by Horseman *et al.* (1996, ch. 10.6)

Soler (1999, 2001) explored the possible importance of coupled processes to repository performance in the affected field. He did this by calculating estimates of the fluid and solute fluxes associated with the coupled processes thermal osmosis, chemical osmosis, thermal diffusion and hyperfiltration, and comparing them with fluxes due to the direct (diagonal) processes advection and diffusion. The conditions were those of a fully saturated Opalinus Clay, at time scales equal to or greater than the expected lifetime of the waste canisters (about 1 000 y). Estimates based on fluxes alone suggest that thermal osmosis is the only coupled transport mechanism that could have a strong impact on solute and fluid transport in the vicinity of the repository. However, when conservation of fluid mass is taken into account in two- and three-dimensional flow models including only advection (Darcy's law) and thermal osmosis, the advective component of flow cancels the thermal-osmotic component arising from the presence of a heat source in the interior of the flow domain. Chemical osmosis would only have a minor effect according to the first estimates. Also, estimates regarding the possible role of thermal filtration and the Dufour effect on heat transport suggest that the effect of these coupled heat transport mechanisms is negligible compared to heat transport by thermal conduction.

43.3 Scaling issues

None reported.

43.4 Scientific level of understanding

Chemical osmosis (FEP 44) and hyperfiltration are well-understood from the point of view of the mechanisms behind the transport phenomena. They are due to the existence of diffuse ionic double layers in solution next to the clay-mineral surfaces. Thermal diffusion (Soret effect) has been studied for many years by many different investigators in different systems. It is well-established as a solute transport mechanism. There is little understanding of the mechanisms underlying thermal filtration and the Dufour effect.

Only two laboratory studies on thermal osmosis in argillaceous material are cited by Soler (1999, 2001). These give values of thermo-osmotic permeabilities from 10^{-14} to 10^{-10} $m^2/K/s$. Soler's calculations show that thermo-osmotic fluxes far exceed advective and diffusive fluxes at thermo-osmotic permeability values much above 10^{-12} $m^2/K/s$. Modelling coupled thermo-osmotic and advective fluxes shows that they cancel leading to very low net fluxes, but to evaluate thermo-osmotic fluxes alone site-specific thermo-osmotic permeability values should be available.

43.5 Linked FEPs

FEP 6 Hydraulic properties of the host rock
FEP 8 Diffusivity
FEP 10 Ion exclusion
FEP 32 Thermal rock properties
FEP 38 Hydraulic properties of the EDZ

43.6 Level of understanding from a PA perspective and treatment in PA

Off-diagonal processes are not included in models used for PA calculations, but can be examined in separate scoping calculations, as was done for the Opalinus Clay. Bounding values for coupled flux parameters may be sufficient to demonstrate that certain processes are not important. If such calculations show that the processes could be important, it may be necessary to measure specific coupling parameters.

Based on current understanding, thermal osmosis is the only off-diagonal Onsager process that could potentially affect the affected-field performance of a repository in the Opalinus Clay. However, further calculations indicate that this too has only a small effect, at least at times beyond canister failure (when the system is likely to be fully saturated). Thermal osmosis may play some role in the resaturation process, but other phenomena are likely to be more important.

On the basis of numerical experiments, it is judged that off-diagonal Onsager processes can be neglected in the formulation of geosphere transport models for Opalinus Clay. The possible role of chemical osmosis in the far field is addressed in FEP 44.

43.7 Available reviews

Coupled processes are not widely studied so each site-specific reference given above in the table in Section II, Chapter 43.2 includes a review of the subject. Those of Horseman *et al.* (1996) and Soler (1999, 2001) are particularly useful.

43.8 Planned work

As shown in the table in Section II, Chapter 43.2 and discussed in FEP 44, laboratory and field work on chemical osmosis and hyperfiltration are under way in connection with site investigations of the Opalinus Clay at Mont Terri, the Callovo-Oxfordian at Bure and the Boom Clay at Mol. No studies of other types of coupling are planned.

43.9 Overall evaluation

Based on the calculations of Soler (1999, 2001), the relevance of off-diagonal processes in the affected field of a repository is low. Thus, further work should be assigned a low priority, although any developments reported in the literature should be followed.

44. CHEMICAL OSMOSIS (FEP B5.5)

44.1 Definition and generalities

Chemical osmosis is the most studied off-diagonal Onsager process. It refers to the fluid pressures or fluxes that develop across a semipermeable membrane in response to a chemical concentration gradient. The converse process, called hyperfiltration, is the process by which solute molecules are prevented by their size and/or charge from passing through a membrane. Hyperfiltration may increase the concentration of solutes within or on the upstream side of a membrane through which a solvent is flowing.

The solvent flux due to chemical osmosis, q, is commonly expressed by an equation analogous to Darcy's law (here written for flow in the x-direction):

$q_\Pi = \sigma\ k/\mu\ \partial\Pi/\partial x,$

and the osmotic pressure, Π, given by

$\Pi = -\ [RT/V_w]\ \ln a_w.$

In the first expression, k = permeability, μ = dynamic viscosity, σ = osmotic efficiency, and ∂Π = loss of osmotic pressure across ∂x. In the second, V_w and a_w are the molar volume and activity of water, respectively, R is the gas constant and T is absolute temperature (Neuzil, 2000, Soler, 1999, 2001).

Scoping calculations, based on properties of the Opalinus Clay and discussed in FEP 43, suggest that chemical osmosis in unlikely to affect the affected-field performance of a repository after resaturation. However, there are four aspects of site characterisation (far field) to which osmosis may be of potential importance:

- as a driving force for fluid flow;
- as a cause of hydraulic overpressures;
- as a cause of erroneous hydraulic pressure measurements due to concentration gradients between borehole and formation fluids; and
- as a thermodynamic potential that affects the geomechanical rock properties (e.g. swelling, mechanical instability).

These potential effects of chemical osmosis are discussed in this FEP.

44.2 Site-specific experimental information

Formation/site	Type of information	Scale	Results and conclusions
Callovo-Oxfordian at Bure	Scoping calculations using salinity contrasts from the field and assumed osmotic efficiency	100 m	Osmosis could explain measured hydraulic overpressures (Tevissen 1999). Site-specific osmotic efficiency yet to be measured. In any case, osmosis is not relevant as a migration mechanism for radionuclides.
Opalinus Clay at Mont Terri (Harrington & Horseman, 1999, 2000; Noy *et al.*, 2003)	Experiments on cores and *in situ* tests in packed boreholes Numerical experiments to assess potential contribution of different off-diagonal Onsager processes to solute fluxes are discussed in FEP 43	cm to m	Laboratory permeabilities were from 7 to 10 x 10^{-21} m^2 with osmotic efficiencies between 1 and 6%. Field experiments gave a consistent osmotic efficiency of 12%.
Opalinus Clay in the Zürcher Weinland (Nagra, 2002, ch. 5.11)	Scoping calculations and numerical experiments based on field measurements	1 to 100 m	Chemical osmosis as a transport process in the Opalinus Clay is negligible due to the absence of strong concentration gradients and due to the limited osmotic efficiency. It cannot explain the observed hydraulic overpressures. Calculations show that chemical osmosis has a negligible effect on the evaluation of *in situ* hydraulic head measurements. Thus test artefacts are excluded.
Pierre Shale in south Dakota (Neuzil, 1994, 2000)	Long-term field experiment	Several 10 m	Fluid pressures and solute concentrations have been measured *in situ* for nine years and showed rapid head change (dm to m per year), which slowed to virtual constancy after 5 to 9 years. The pattern could be quantitatively interpreted as an initial pressure change due to chemical osmosis which slowed down as diffusion lowered the concentration gradient. The relative importance of diffusion demonstrates that the osmotic membrane is not ideal.

44.3 Scaling issues

None reported.

44.4 Scientific level of understanding

Chemical osmosis is well-understood from the point of view of the mechanism behind the transport phenomenon. However, quantitative modelling of the effect of osmosis within a natural argillaceous formation (i.e. a complex mixture of different clay minerals) is rather poorly understood, among other reasons due to the scarcity of measurements of osmotic efficiency.

44.5 Linked FEPs

FEP 6	Hydraulic properties of the host rock
FEP 8	Diffusivity
FEP 10	Ion exclusion
FEP 17	Pore- and fracture water composition
FEP 38	Hydraulic properties of the EDZ

44.6 Level of understanding from a PA perspective and treatment in PA

The effects of chemical osmosis in the affected field are negligible. Similarly, it is considered to be irrelevant as a transport process for radionuclides in the far field. For these reasons, chemical osmosis is currently neglected in PA. Few data exist regarding osmotic efficiency of argillaceous rocks but appear to indicate that such rocks are only non-ideal membranes.

On the other hand, chemical osmosis is a possible explanation of hydraulic overpressures observed in some argillaceous formations, and thus needs attention from a viewpoint of site characterisation and system understanding. It may also be considered in the evaluation of hydraulic head measurements in boreholes, in particular if the test fluid has a salinity that is substantially different from that of the *in situ* pore-water.

44.7 Available reviews

Horseman *et al.* (1996).

44.8 Planned work

None reported.

44.9 Overall evaluation

This process can be neglected in comparison with other transport processes and need not be implemented in models used for PA.

However, laboratory and field evidence show that chemical osmosis due to natural or introduced concentration gradients can produce anomalous pressures. Such pressures could lead to misunderstanding of the hydraulic heads driving regional flow, to incorrect interpretations of hydraulic head measurements in boreholes, and to mechanical instability in boreholes and underground workings from osmotic pressures developed in the formation.

45. GAS DISSOLUTION AND CHEMICAL INTERACTIONS BETWEEN GAS AND PORE-WATER (FEP B6.1)

45.1 Definition and generalities

This FEP is concerned with gases dissolved in the pore and fracture water *in situ* and the dissolution of gases present during the operational phase of the repository and/or from degradation of parts of the engineered barrier system. It further addresses the chemical interactions that might occur between pore-water and gases. In is relevant to the affected field in connection with the EDZ

The solubility of a gas depends on the partial pressure of the gas and its temperature-dependent Henry's Law or other gas law constants. In a closed system (a system with a limited total gas volume) the dissolved concentration also depends on the volume ratio of solution to total gas (Stumm & Morgan, 1996). Henry's Law constants are commonly included in the thermodynamic data bases used for geochemical modelling (see FEP 22). Other forms of gas solubility data (e.g. IUPAC or van der Waals expressions) are summarised in handbooks (e.g. Lide 1994).

The identities and availability of the dissolved gases must be known to address this FEP. This information will come from knowledge of the chemistry of pore-water *in situ*, and from consideration of repository construction and operation procedures and of the waste products and other materials present in the repository. Repository operation and materials are beyond the scope of this FEP.

45.2 Site-specific experimental information

The composition of *in situ* pore-water, including its dissolved gases, has been determined for a number of potential argillaceous host rocks and other argillaceous formations. These are tabulated in Section II, Chapter 17.2.

Dissolved gas analyses have been carried out for several field experiments in the Boom Clay, namely CERBERUS (Noynaert *et al.*, 1998a) and CORALUS (Valcke *et al.*, 1999b). All these experiments refer partially to the release of gases (by anaerobic corrosion, radiolysis, thermal decomposition, microbial activity) into the Boom Clay, but do not directly address the process of gas dissolution.

Laboratory experiments on gas diffusion and reaction in Boom Clay have been carried out in the frame of the MEGAS (Volckaert *et al.*, *1*995 & Ortiz *et al.*, 1997) and the PROGRESS projects (Rodwell 2000). In batch reaction experiments, hydrogen was put in contact with a Boom Clay slurry, prepared with fresh clay and with either pure or synthetic clay water at ambient temperature. The pressure evolution in the continually stirred reactor was monitored. According to the pressure evolution, it takes only a few hours for the gas to dissolve in the clay slurry. The quantities of dissolved gas corresponded more or less to the theoretical solubility data in pure water. During these experiments with hydrogen, the microbiological conversion of hydrogen to methane was observed (see also FEP 49).

For the diffusion experiments, a gas phase (hydrogen or methane) is put in contact with fresh Boom Clay samples. Either the consumed gas volume at the inlet under isobaric conditions or the pressure evolution at the outlet was monitored. From these results, the diffusion parameters were calculated with an analytical model. In the conceptual model, it was assumed that the solubility of gas corresponded to the theoretical solubility data in pure water and that Henry's Law was valid.

45.3 Scaling issues

None reported. The dissolution and reaction processes are global.

45.4 Scientific level of understanding

Gas dissolution and other equilibrium reactions and the diffusional transport of dissolved gases are well understood. They can be satisfactorily predicted if site-specific boundary conditions are known. The kinetics of gas reactions, like those of all reactions, are less well known. If the site is heated, by radioactive decay of waste or by a shifting geothermal regime, gas solubility will decrease and a separate gas phase may appear. The parameters governing gas transport are generally less well known.

While the processes are reasonably well understood, there are uncertainties in site-specific gas-concentration data and in knowledge of the identities and rates of production of gases within the repository.

45.5 Linked FEPs

FEP 17	Pore- and fracture water composition
FEP 22	Thermodynamic and kinetic modelling data
FEP 26	Oxidation of the host rock
FEP 49	Microbiological perturbations

45.6 Level of understanding from a PA perspective and treatment in PA

The solubility and transport properties of any gaseous radionuclides (e.g. Iodine) are known. Gas dissolution and reactions are not modelled directly in PA. However, in order to calculate the transport capacity of dissolved repository gases by advection and diffusion, the pressure- and temperature-dependent gas solubilities are required as input, plus knowledge of possible chemical reactions that could affect transport capacity. Thus the role of this FEP lies in the assessment of the relevant gas transport mechanisms, which is a basis for more detailed modelling of these mechanisms in the framework of PA.

45.7 Available reviews

Modelling gas dissolution and reactions are discussed in any textbook of geochemistry. Gas transport is reviewed by Rodwell *et al.* (1999).

45.8 Planned work

None reported.

45.9 Overall evaluation

Gas dissolution and reactions in solution are included in the geochemical site characterisation activities and modelling carried out in support of the sorption FEPs 17-22 (A2.2 series). They are also considered in the assessment of the relevant transport mechanisms for repository-derived gas.

46. GAS MIGRATION THROUGH THE PRIMARY POROSITY (MATRIX, NATURAL FRACTURES) (FEP B6.2)

46.1 Definition and generalities

The amount of gas generated within a repository depends on two main factors: (a) the total amount of organic materials and compounds contained within the repository that are prone to chemical and biological degradation, and (b) the amount of corrodible metals (e.g. iron, carbon steel, aluminium) present in the wastes, used in the manufacture of waste containers, or utilised in repository construction. Although gases are also generated by radioactive decay of the waste and by the radiolysis of water and other compounds, the total amount is generally very small. The gas generation rate depends on the waste composition and on the materials selected for waste containers and repository construction.

Gas migration processes include:

(a) diffusion of gas molecules in water,

(b) advection of water containing dissolved gas,

(c) movement of gas as a discrete phase within the original (or primary) pore space of the material,

(d) movement of gas as a discrete phase within natural fracture porosity of the material,

(e) movement of gas as a discrete phase within stress- or pressure-induced microscopic porosity in the rock matrix (pathway dilation),

(f) movement of gas as a discrete phase within stress- or pressure-induced macroscopic fractures (gas fracs).

In processes (a) and (b), no separate gas phase is present and gas transport can be described by the convection-dispersion equation (single-phase liquid flow). These processes will be dominant as long as the gas generation rate is lower than the diffusive and advective flux of dissolved gas, and they are addressed in FEP 45. In processes (c) and (d), a separate gas phase is formed in the existing pore space and two-phase flow will occur. These processes are dealt with in this FEP. Two-phase flow is an advection process in which two separate phases (water as a wetting fluid and gas as a non-wetting fluid) flow at the same time through a poro-elastic geological medium. Two-phase flow can be described by the extended Darcy law in which the flow of each phase is determined by its respective pressure, density and viscosity. In process (e), gas migration occurs through dilated pores in the rock matrix. The evidence of microscopic dilation is mainly the observation that gas permeability of the sample is pressure-dependent. No macroscopic fractures are developed in this process, and the two fluids interact in a similar way as in processes (c) and (d), thus it can also be regarded as two-phase flow. Process (f) involves the creation of a macroscopic fracture where single-phase transport of gas occurs. Processes (e) and (f) are treated in FEP 47.

There is substantial evidence suggesting that gas migration in the far field is likely to be focused along faults and fractures, if these are present in the formation. Soil-gas surveys show that vertical gas movement through low-permeability sequences is associated with major structural geological features, and it is sometimes feasible to infer the location of such features from contoured plots of gas concentration. Studies aimed at improving the production of natural gas from shale reservoirs have also emphasised the importance of fractures in controlling gas migration.

46.2 Site-specific experimental information

Formation/site	Results and conclusions
Opalinus Clay at Mont Terri (experimental data)	Tests on disturbed and undisturbed samples were performed in oedometric conditions in the laboratory (Ortiz Amaya, 2000). Gas entry pressures were 0.5 MPa or less, i.e. substantially lower than confining pressure (6 MPa; hydrostatic pressure = 2 MPa). Expulsion of water was observed, indicative of interactions between the fluid phases and thus of two-phase flow through the rock matrix. *In situ* tests in the underground research laboratory: Marschall *et al.* (2003), Croisé *et al.* (1999). The *in situ* gas threshold pressure test could be simulated using a classical two-phase flow model; further simulations were done including a coupling between fluid flow and geomechanics at the cost of an increase of the number of parameters, of which the independent determination is very difficult. With both approaches, the pressure evolution in the injection test interval could be correctly simulated. However, the simulation of the responses in the cross-hole tests remains problematic.
Opalinus Clay at Mont Terri and in the Zürcher Weinland (concepts and interpretations)	The transport capacity of advective and diffusive transport of gas dissolved in pore-water (alternatives a and b above) is very limited and not sufficient to accomodate the expected gas production rates. Migration of gas as a discrete phase in the primary porosity (i.e. classical two-phase flow, alternative [c] above) is controlled by the capillary gas entry pressure. This parameter has been investigated for Opalinus Clay through *in situ* gas threshold pressure tests at Mont Terri and in the Benken borehole and by gas permeability tests with core specimens from both sites. The determined entry pressures were in the range of 1-10 MPa (values around 1 MPa at Mont Terri, up to 10 MPa in the Benken borehole). Comparing these values to the expected gas production rates, it is concluded that a significant part of gas will be transported in the connected system of natural macropores (equivalent radii > 25 nm) of the rock matrix. Microstructural analyses of the Opalinus Clay at Benken yield a total porosity of 0.11, whereby the fraction of macropores amounts to 20%. Pathway dilation (FEP 47) is also expected to contribute to gas transport in Opalinus Clay, while the creation of macroscopic gas fracs are very unlikely. References: Marschall *et al.* (2003), Nagra (2002).

Formation/site	Results and conclusions
Boom Clay at Mol	Laboratory tests on Boom Clay cores and *in situ* tests in the underground research laboratory showed clearly that gas flow in Boom Clay does not occur through the primary porosity but exclusively through stress-induced porosity (Volckaert *et al.*, 1995, Ortiz *et al.*, 1997, Rodwell *et al.*, 1999). This is demonstrated by the observation that the gas injection rate varies exponentially with pressure.
Other: Soil gas surveys and gas injection tests in faulted argillaceous formations	Studies show that gas flow is often very localised and dominated by a small number of hydraulically active fractures. A field gas injection test also showed that the connectivity of faults has a large influence on the pathway followed by the gas (Lombardi *et al.*, 1996, Durrance *et al.*, 1989).

46.3 Scaling issues

Upscaling of two-phase flow properties, especially for fractures, to repository dimensions is difficult. Scaling in time is also an issue, as laboratory experiments or *in situ* tests are conducted over short time scales. Gas fracs observed in such experiments may not develop in a repository situation where pressure build-up is much slower and gas transport can possibly be accomodated by two-phase flow (whether through the primary porosity or through dilated pathways).

46.4 Scientific level of understanding

Darcy-type two-phase flow in porous media is a scientifically well understood process and several numerical codes (e.g. TOUGH2, CODE-BRIGHT) are available (Manai, 1997).

46.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 6	Hydraulic properties of the host rock
FEP 9	Connected matrix porosity
FEP 35	Size and structure of the EDZ
FEP 38	Hydraulic properties of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 42	Self-sealing
FEP 55	Present-day stress regime

46.6 Level of understanding from a PA perspective and treatment in PA

As the generation of substantial quantities of gas is highly probable in most repository designs, the explicit treatment of gas migration in PA is required. In some repository systems, a substantial part of the gas transport capacity is accomodated by two-phase flow in the primary porosity, which is not the case for other systems where stress-induced pore spaces are important. The relevant gas-transport mechanism is also strongly determined by the considered gas generation rates, which depend on waste composition, repository design and the degree of conservatism in the choice of corrosion rates, e.g. those of metals.

46.7 Available reviews

Rodwell *et al.* (1999), Rodwell (2000), NEA (2001).

46.8 Planned work

At the EC level, the thematic network GASNET was started to discuss how to treat gas issues in safety assessment.

46.9 Overall evaluation

The relevance of gas migration through the primary porosity varies among disposal concepts, especially the expected gas generation rates, host formations and approaches to interpret experimental findings.

47. GAS MIGRATION THROUGH STRESS-INDUCED POROSITY (GAS FRACS, PATHWAY DILATION) (FEP B6.3)

47.1 Definition and generalities

An overview of all gas-migration mechanisms is given in Section II, Chapter 46.1.

In the case that the rate of gas migration through the primary porosity (FEP 46) is smaller than the gas production rate, a gas-pressure-driven dilation of pre-existing (preferential) pathways or the spontaneous formation of new fractures (“pneumatic fracturing”, “gas fracs”) will occur. The geometry of the pre-existing pathways may be linear (pipes) or planar (planes). Pneumatic fractures are always planar.

Pathway dilation: Considering the micro-scale variability of the rock strength, it is plausible that microfractures will form prior to any macroscopic fractures, and this process is termed pathway dilation (Horseman *et al.* 1996). For pathway dilation to occur, the gas pressure must exceed the local normal stress component acting across the plane that is being dilated. This microscopic fracturing causes an increase of the pore space (dilatancy), and a detectable increase of intrinsic permeability. While the regime of the conventional two-phase flow sees the intrinsic permeability quasi independent of the absolute gas pressure, for pathway dilation related to microscopic fracturing the permeability is observed to increase with increasing gas pressure. Pathway dilation typically occurs when the gas pressure is allowed to increase slowly: additional pore volume – which is the result of dilation – is created at a rate which coincides with the gas production rate. A quasi-stationary gas flow may thus evolve along the newly opened gas flow path.

Pneumatic fracturing, formation of gas fracs: Pneumatic fracturing is identical to common hydraulic fracturing with the only difference that it is caused by an over-pressured gas instead of a liquid. For pneumatic fracturing to occur, the gas pressure must exceed the minor principal stress σ_3 acting in the host medium plus the tensile strength of the medium (Fioravante *et al.*, 1998). This critical gas pressure is known as the “frac pressure”. A macroscopic frac typically develops when the gas pressure build-up is rapid, i.e. when the gas production rate is no longer matched by the formation of microscopic fractures (dilatancy). A macroscopic frac is initiated quasi-instantaneously and propagates in a plane which is oriented normally to the direction of σ_3. The propagation comes to a halt when the gas pressure in the macroscopic fracture becomes less than the value of the minimum principal stress (shut-in pressure). When the gas pressure is increased once more, the re-frac pressure is reached when the previously created fracture is re-opened. The value of the re-frac pressure is intermediate between shut-in pressure and frac pressure. The conceptual, theoretical and experimental framework for fracture propagation is well documented in standard hydrocarbon exploration literature (Valko & Economides 1997). Gas transport in a tensile fracture occurs as a single phase gas flow. The phase interference with the pore-water is – in a first approximation – negligible.

The extent to which pneumatic fractures may propagate into the host rock is important for PA, as pneumatic fractures might become preferential pathways for the repository fluids and could short-cut the barrier function of the host rock.

47.2 Site-specific experimental information

Formation/site	Results and conclusions
Opalinus Clay at Mont Terri (experimental data)	*Laboratory experiments:* Rummel *et al.* (1998). *In situ in the underground research laboratory:* (1) Gas-frac self-sealing experiment: An artificial fracture was hydraulically induced and subsequently re-opened by gas-pressure-induced flow (Enachescu *et al.*, 2002). (2) Based on the Mont Terri field data, some conceptual models for gas flow were developed in which pneumatic fracturing could be of some importance (Fisch & Piedavache, 2000; Fierz, 2000). Dilative strain was measured in observation intervals during gas testing in the framework of the GP-Experiment (Marschall *et al.*, 2003). The observations are in agreement with the formation of some gas-pressure-induced artificial microfractures.
Opalinus Clay at Mont Terri and in the Zürcher Weinland (concepts and interpretations)	Qualitative and quantitative evidence for dilatant gas transport mechanisms at gas pressures below minimum principal stress (σ_3) was gained mainly through a series of *in situ* experiments at Mont Terri (see above). Experimental evidence for pathway dilation includes pressure-dependent permeability at elevated gas pressures and significant volumetric strains during gas injection tests (laboratory and field tests). In any case, clear evidence for phase interference was seen (water expulsion). Hydraulic tests before and after the *in situ* gas tests did not show significant changes of hydraulic conductivity of the rock mass due to the injection. It is concluded that pathway dilation is a relevant process and, together with classical two-phase flow (FEP 46) accounts for the transport of gas generated in a repository in Opalinus Clay, while gas fracs are not expected to be generated. The transition between the two processes is not sharp - due to the high gas entry pressures, the onset of microscopic pathway dilation during pressure build-up may be expected before water displacement starts. In fact, both gas transport processes will not give rise to significant alteration of the rock properties (e.g. enhancement of intrinsic permeability) during the passage of a gas phase. At Mont Terri, hydraulic fracs and gas re-fracs were created. Frac pressure was surprisingly high at about 9 MPa and refrac pressure was approximately 5 MPa. References: Marschall *et al.* (2003), Nagra (2002).

Formation/site	Results and conclusions
Boom Clay at Mol	*In situ tests in the underground research laboratory:* Several gas injection experiments in three different experimental setups: (1) Volckaert *et al.* (1995): A chain piezometer was installed in a vertical borehole. Gas (helium) injection tests were carried out in two sealed borehole sections at depths of 7 and 13 m. In both cases, a pneumatic breakthrough occurred along the borehole walls at lower pressures than expected. Explanation: Local disturbance of the geomechanical stress field by the existence of the drill hole. (2a) Chain piezometers were installed in four horizontal boreholes. Repetition of the observation made in the vertical borehole. (2b) Ortiz *et al.* (1997): A hydraulic fracturing test was carried out four months after a gas injection test in the same borehole section. The hydraulic conductivity was found to be identical with that of the undisturbed clay (1.57 x 10^{-12} m/s). This gives evidence of the self-sealing capabilities of the clay (see also FEP 42). (2c) Rodwell (2000): A gas pathway was created between two sealed sections and kept open for a time span of 1 year. A HTO injection was subsequently carried out in one of the sections and the HTO dissipation process monitored in the source and adjacent sections. The result was that the former gas pathway did not act as a preferential pathway for the migration of radionuclides. (3) Volckaert *et al.* (2000): Sealing tests in a horizontal borehole using two different types of bentonite seals (FoCa Clay and Serrata Clay). A pneumatic breakthrough was observed along the borehole walls at a gas overpressure of 1.5 MPa. This pressure is equivalent to the radial stress developed within the seal. This observation proves that the formation of gas pathways is stress-controlled. *Laboratory tests* yielded substantial information on the controlling mechanisms of gas migration through Boom Clay (Volckaert *et al.*, 1995; Ortiz *et al.*, 1997; Rodwell *et al.* 1999 and Rodwell 2000). The main results are the following: • The gas injection rate varies exponentially with pressure. This definitively precludes any Darcian behaviour. • The gas breakthrough pressure is about inversely proportional to the cubic root of the hydraulic conductivity of the sample. • The presence of residual gas in the clay lowers both the gas entry and the breakthrough pressure when the clay is submitted to a second cycle of gas injection. *Numerical and conceptual models:* A variety of models were developed in connection with the MEGAS and PROGRESS projects. The most noticeable models are as follows: • 1-D two-phase flow code TOPAZ (Worgan 1992; Worgan and Impey 1992). Results: Good prediction of the steady-state behaviour, however not of the

Formation/site	Results and conclusions
	transient behaviour. The breakthrough times were grossly over-estimated. As a consequence the rock compressibility effects were incorporated into the model (Impey *et al.*, 1993). This gave successful predictions and good agreement with experimental results. • "Capillary Bundle Model" (Einchcomb & Impey, 1995a, b). This model is based on an idealised, topological representation of gas-water migration pathways. Good agreement between numerical and experimental results supports the hypothesis that preferential pathways play a significant role in gas migration through Boom Clay. • Mathematical model to predict the propagation of gas pathways through an argillaceous medium (Einchcomb & Impey, 1997). A simple micro-mechanical model to be applied to Boom Clay was introduced. A key feature of this model is that it contains parameters which control the dependence of the pathway propagation and dilatation on the gas pressure and boundary conditions. The choice of these parameters may depend on the stress field. The predictions are qualitatively similar to the experimental results. The drawback of the model is that it needs a lot of input data which are difficult to obtain experimentally. • Conceptual model to simulate the thermo-hydro-mechanical behaviour of unsaturated soil (Olivella *et al.*, 1994). The model correlates the mechanical properties of the soil with gas pressure and flow evolution. More recently, a new procedure was implemented which generates random fields to simulate soil heterogeneity for input data to the model.
Various	Soil gas surveys and gas injection tests in faulted argillaceous formations.

47.3 Scaling issues

Repository gas migration raises a wide range of issues associated with the upscaling of experimental findings from the laboratory and borehole scales to the scale of the formation. The single most important issue is the likely role of preferential pathways (e.g. EDZ fractures, dilatant fault zones, gas fracs) in the gas migration process.

Upscaling of laboratory-scale experimental results to repository dimensions in space and time is difficult and subject to ongoing debate. With regard to the Boom Clay there is the opinion that the information obtained in the lab and in the underground research laboratory can be upscaled to the whole Mol site.

47.4 Scientific level of understanding

Knowledge of gas-entry pressures into the matrix of argillaceous media is limited. At least in some cases, this pressure is significantly lower than the minimum compressive stress component of the *in situ* stress field, and indications exist that gas flow takes place in diffuse dilated pathways in the matrix (and not in a macroscopic gas frac that would develop if the gas entry pressure exceeds the minimum stress; see Nagra, 2002).

Flow of gases along dilated pathways in argillaceous material has been modelled by AEAT for the GAMBIT consortium (Swift *et al.*, 2001; Horseman *et al.*, 1999). A multiple front propagation model for gas migration in plastic clay is described by Brown (1999).

The basic principles of pneumatic fracturing are well established. In contrast, at the microscopic scale there is a conspicuous lack of knowledge on the initiation and propagation of pneumatic fractures in saturated low-permeability argillaceous formations. Theoretically, the threshold capillary pressure for gas entry into the extremely narrow water-filled space is far beyond the pressures which are common in geotechnical applications. The discrepancy between practical evidence on the macroscopic scale and theoretical considerations of the microscopic level may be explained by the existence of small discrete features, in particular cracks, which give rise to major local stress concentrations.

47.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 6	Hydraulic properties of the host rock
FEP 35	Size and structure of the EDZ
FEP 37	Geomechanical rock properties
FEP 38	Hydraulic properties of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 42	Self-sealing
FEP 55	Present-day stress regime

47.6 Level of understanding from a PA perspective and treatment in PA

As the generation of substantial quantities of gas is highly probable in many repository designs, the explicit treatment of gas migration in PA is required. Simplified assessments have already been performed in several countries (see NEA, 2001).

With regard to pneumatic fracturing, the underlying processes are qualitatively well understood, however not yet adequately mastered for quantitative modelling. It remains a difficult task to fully and globally predict its influence at the repository scale.

For the Boom Clay, preliminary simplified PA studies (Volckaert & Mallants, 1999; Mallants & Volckaert, 1999) indicate that gas generation and gas migration may not be overly problematic, although the conclusions remain subjected to simplifying, conservative hypotheses. Three cases have been investigated for high- and medium-level waste as follows: (1) No influence of the generated gas on the hydraulic regime; (2) Movement of a gas/water interface in upward direction (Darcy flow); (3) Gas flows through the argillaceous formation via a hydrofracture. One result of these studies is that gas generation and migration can quantitatively influence the predicted release of the non-retarded radionuclides through the expulsion of contaminated water in the case of medium-level waste. However, these studies were carried out assuming simplified conditions due to the lack of information on the characteristic curve (saturation in function of gas pressure) of the backfill and on the effective porosity of the hydrofracture.

In Opalinus Clay of the Zürcher Weinland, gas fracs are not likely to occur (Nagra, 2002). The transport capacity of classical two-phase flow (i.e. through the natural pore space, FEP 46), possibly with a contribution of transport along dilated pathways, appears to be sufficient to prevent the build-up of excessive gas pressures.

It has been suggested to alleviate the potential problems of gas over-pressurisation by installing a vent which would let the repository gas escape to the atmosphere without enhancing the migration of the radionuclides. The technical feasibility of such a solution needs careful investigation.

47.7 Available reviews

Generic: Rodwell *et al.* (1999); Rodwell (2000); NEA (2001).

47.8 Planned work

Opalinus Clay at Mont Terri, GP-B Experiment: Gas and water coupled processes. The experimental basis of this experiment relates to the observation of the longer-term response of cracks in the EDZ to stress changes imposed in boreholes.

At the EC level the thematic network GASNET was started to discuss how to treat gas issues in safety assessment.

47.9 Overall evaluation

Gas migration through stress-induced porosity is regarded as a highly relevant FEP which is qualitatively rather well understood. However, current understanding is not yet sufficient for detailed quantitative assessments mainly due to questions on the most relevant type of preferential pathway and on the effects of geomechanical coupling.

Calculations suggest that this FEP should not pose a threat to the global safety of a repository. However, some strongly simplifying hypotheses were made in these calculations thus underlining the remaining importance of this FEP.

The issues associated with gas movement in argillaceous host rocks have close parallels with those that arise when examining gas flow in clay-based buffers, backfills and seals. The gas migration processes discussed above are also applicable to the clay components of the engineered barrier system.

48. GAS-INDUCED TRANSPORT IN WATER (FEP B6.4)

48.1 Definition and generalities

When a gas phase is formed in a water saturated repository system, water will be expelled from it. If gas generation from a repository is such that substantial pressure build-up occurs, intermittent gas flow can occur. Flow of gas is associated with a gas-driven transport of water. Both processes can lead to a gas-induced transport of radionuclides in water.

48.2 Site-specific experimental information

Formation/ site	Type of information	Scale	Results and conclusions
Opalinus Clay at Mont Terri	Gas injection tests on cores	cm	Tests on a disturbed and on an undisturbed sample were performed in oedometric conditions. Only very small quantities of water were displaced by gas intrusion and flow (degree of desaturation 7% for an undisturbed sample; Ortiz Amaya, 2000).
Boom Clay at Mol	Gas injection tests on cores	cm	Evidence of instability of gas pathways and pulse-type gas flow. Only very small quantities of water are displaced by gas intrusion and flow (degree of desaturation < 3%; Ortiz *et al.*, 1997).
Other	Soil gas surveys and gas injection tests in faulted argillaceous formations	m to km	Gas pathways and conductivity of faults indicate non-continuous gas flow. No estimation of water displacement available (Lombardi *et al.*, 1996, Durrance *et al.*, 1989).

Laboratory experiments showed that gas pathways, especially in plastic clays, are highly unstable. Even at constant gas pressure the gas flow is not continuous. Gas pathways collapse and reopen frequently and are extremely sensitive to small fluctuations in fluid pressures and mechanical stress. Water flow associated to the gas flow is very small.

Soil gas surveys show a link between gas flow and major faults. There are indications that in the case of bubble flow in open fractures, transport of particles at the bubble-water interface could contribute to the global mass transport (Lombardi *et al.*, 1996).

48.3 Scaling issues

Upscaling of experimental findings from the laboratory and borehole scales to the scale of the formation and the waste repository is very difficult.

48.4 Scientific level of understanding

Although the fundamental processes are rather well understood, understanding is still insufficient for large (repository) scale modelling and parametrisation.

48.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 6	Hydraulic properties of the host rock
FEP 37	Geomechanical rock properties
FEP 38	Hydraulic properties of the EDZ
FEP 39	State of saturation of the EDZ and desiccation cracking
FEP 42	Self-sealing
FEP 46	Gas migration through the primary porosity (matrix, natural fractures)
FEP 47	Gas migration through stress-induced porosity (gas fracs, pathway dilation)
FEP 55	Present-day stress regime

48.6 Level of understanding from a PA perspective and treatment in PA

When a gas phase is formed in a water saturated repository, pressures develop and water will be expelled. This water can be contaminated if the waste packages are already being leached. The potential of the whole process to increase radionuclide transport from a repository depends on the relative kinetics of the resaturation of the repository after closure, the evolution of the structure and permeability of the EDZ, the rate of gas generation, the rate at which waste containers start to leak and the leaching rate of leaky containers. The coupling between these processes makes the modelling or the assessment of their global influence on radionuclide transport complex.

Examples of the treatment of gas-induced radionuclide transport in water in PA can be found in NEA (2001). In general, these assessments are performed in a simplified conservative way, in order to assess the potential for an increased radionuclide transport. Under some very site-specific combinations of the mentioned processes, an increase in the transport of some radionuclides is possible. However, the influence on the overall repository system is low.

48.7 Available reviews

NEA(2001), Rodwell *et al.* (1999).

48.8 Planned work

At EC level, the thematic network GASNET was started to discuss how to treat gas issues in safety assessment.

48.9 Overall evaluation

In principle, gas-induced transport of water can increase the radionuclide flux to the biosphere, because this process can short-cut the barrier function of argillaceous host rocks. Therefore it is a highly relevant FEP. The quantitative evaluation of this FEP is very complex due to the coupling with hydro-mechanical, gas-generation and waste-leaching processes. Detailed modelling is currently not possible due to the difficulty of upscaling experiments to repository level and due to the lack of reliable large-scale models and parameters. However, preliminary assessments indicate that the overall effect on repository safety would be rather small or even negligible.

49. MICROBIOLOGICAL PERTURBATIONS (FEP B7)

49.1 Definition and generalities

Microbiological perturbations include the effects of microbes or changing microbe activity on host-rock properties and on radionuclide transport. Microbes introduced into the repository system may enhance the rates of some chemical reactions, or they induce reactions that would not occur in an abiotic environment. Microbes may sorb radionuclides and act as colloids. Gas production, e.g. methane, causing a possible build-up of a gas phase in a repository is also of concern.

49.2 Site-specific experimental information

The information provided as the basis for this section describes studies intended to identify microbes present in the formations and waters sampled rather than the perturbations caused by these microbes.

Formation/ site	Type of information	Results and conclusions
Boom Clay at Mol	Clay samples	Sulfur oxidising and reducing bacteria, methanogenic bacteria were identified (Ortiz *et al.*, 2002).
Boda Clay Formation at Mecsek	Air, ground water, rock and technological water samples taken from the underground research laboratory	Aerobic (about 10^5 culture initiations/ml) and anaerobic (about 10^3 culture initiations/ml, $>10^6$ culture initiations/ml in technological waters) acid producing bacteria. In one rock sample sulfate reducing bacteria could be indentified. In technological waters sulphate reducing and hydrogen generating bacteria were identified and are unambiguously a product of human drag-in.
Mizunami Group at Tono	Ground-water samples from boreholes	10^7 cells/ml in sedimentary rocks to 10^6 cells/ml in granites, large number of anaerobic bacteria expected in an underground environment.
Generic and bentonite-specific (review by Stroes-Gascoyne, 2002)	Generic observations and experiments with bentonite	Bacteria generally have diameters ranging from 0.1 to a few µm. The mostly much smaller pores in argillaceous rocks would be expected to greatly restrict the ability of bacteria to move and reproduce effectively. Measurements of microbial populations show that sands/sandstones have the highest and argillaceous lithologies the lowest microbial populations (Chappelle, 1993). Apart from size constraints, the limited availability of free water in bentonite and argillaceous lithologies precludes bacterial life (a substantial part of the water molecules in the pore space are bound on mineral surfaces or in hydration spheres of ions).

Bacterial effects are not well studied, and the experimental data base is very small. In argillaceous rocks, the pore sizes in the matrix are often too small for organisms, with the possible exception of faults and fractures. However, bacteria are most likely present in the affected field where open spaces of adequate size may be abundant. It is difficult to determine whether they were originally present or introduced due to the excavation works. Generally, molecular (e.g. PCR) techniques show that many more genera of micro-organisms are present than can be cultivated.

49.3 Scaling issues

None reported.

49.4 Scientific level of understanding

During construction and operation, the whole repository will be contaminated with a wide variety of micro-organisms. Some of these can survive under very harsh conditions. Little is known about what will happen during the transient phase when the geochemical system evolves from an aerobic to an anaerobic atmosphere. It is however clear that when micro-organisms have very little access to space and nutrients, their activity and mobility will be very limited.

49.5 Linked FEPs

FEP 9	Connected matrix porosity
FEP 15	Natural organics, complexation
FEP 17	Pore- and fracture water composition
FEP 30	Organics from waste and their effect on transport properties of the host rock
FEP 42	Self-sealing

49.6 Level of understanding from a PA perspective and treatment in PA

From a PA perspective, the importance of bacterial activity is mainly related to the influence on gas generation by bacterial degradation of organic materials in medium-level waste, the chemistry of the affected field and the possible influence on container corrosion. From the point of view of radionuclide migration in the host rock, micro-organisms probably play a very limited role due to the small pore size in argillaceous formations and the limitation of mass transport to the diffusion mechanism in several (but not all) argillaceous systems.

In actual PAs, this FEP has been only considered in connection to gas generation to date.

49.7 Available reviews

None reported.

49.8 Planned work

An experiment dealing with microbiology is planned for the coming investigation phase (2003-2004) in the Mont Terri underground research laboratory.

49.9 Overall evaluation

Issue important for gas generation from organic materials in medium-level waste. Very little is known about this FEP, and there is no consensus on its (ir)relevance.

50. PAST BURIAL HISTORY (FEP C1.1.3)

50.1 Definition and generalities

Burial history includes all events and processes that affected a formation since the time of sedimentation. In specific, it includes vertical movements (burial, uplift), compaction and expulsion of pore-water, diagenesis, stress and thermal history, and deformation events.

50.2 Site-specific experimental information

Formation/ site	Results and conclusions
Callovo-Oxfordian at Bure	The formation was subjected to burial throughout the Mesozoic, with only minor effects of uplift since the Tertiary. Maximum temperatures in the formation are estimated at 50°C.
Toarcian-Domerian at Tournemire	Since sedimentation, the Jurassic and Early Cretaceous evolution was characterised by extension and subsidence of the basin. Calcite veins precipitated during this period. This stage was followed by a basin inversion that began 90-110 Ma b.p. and led to the erosion of 800-1600 m of Cretaceous sediments. A compressive stage occurred during the Eocene (Pyrenean orogeny). Temperature history was reconstructed by the study of fluid-inclusions, Rock-Eval pyrolysis of organic matter, apatite fission tracks and clay mineralogy. Maximum temperatures during burial are estimated at 80-120°C. Calcite veins that crystallised during the Pyrenean stage indicate temperatures of formation of 30-40°C (evidence from fluid inclusions). Reference: Peyaud (2002).
Opalinus Clay at Mont Terri	Similar to the Zürcher Weinland, Opalinus Clay at Mont Terri experienced a two-stage burial and uplift history (Nagra 2002). The first burial occurred in the Cretaceous and resulted in an estimated overburden of 1 350 m and temperatures comparable to those of the Zürcher Weinland (see below). The second, Miocene burial event was more weakly developed than in the Zürcher Weinland (estimated depth of Opalinus Clay *ca.* 1 000 m) because less deposition of Molasse sediments occurred. However, major uncertainties regarding the thickness of (now eroded) Cretaceous and early Tertiary sediments remain. Thus unlike in the Zürcher Weinland, the first, Cretaceous burial at Mont Terri resulted in both maximum burial and maximum temperature ever experienced by the formation.

Formation/ site	**Results and conclusions**
	In detail, the Tertiary evolution can be described as follows (Wermeille & Bossart 1999): • In the early Oligocene (37-28 Ma), the area is under shallow marine conditions (Lower Marine Molasse). Formation of N-S faults east of St. Ursanne and creation of the Mont Terri flexure (in the context of the Rhine Graben). • Continued subsidence of the Delémont basin, deposition of the Lower Freshwater Molasse (lacustrine and river sediments, 28-21.5 Ma). • Continued subsidence between 21.5 and 10.5 Ma. The area around St. Ursanne is emerged and hydrologically separated from the Delémont Basin. Starting of the erosive period and formation of the Doubs river valley. • The folding of the Jura Mountains occurs in the period 10-3 Ma and is related to uplift and erosion. Aquifers above and below the Opalinus Clay start receiving modern recharge. • Eight glaciation phases between 2 Ma and 13 000 a occurred. The front of the maximum glaciation, which occurred 780 000 a b.p., lies about 10 km south of St. Ursanne.
Opalinus Clay in the Zürcher Weinland	A number of different techniques were used to characterise the burial and temperature history of the sedimentary rocks of the Zürcher Weinland, including studies of stratigraphy, fluid inclusions, clay mineralogy, petrography of cements, vitrinite reflectance, biomarkers (incl. pyrolysis experiments), fission tracks in apatite, shale compaction and basin modelling (Nagra, 2002). Stratigraphic evidence suggests that the Opalinus Clay was subjected to two successive events of burial and uplift, and it is currently over-consolidated (OCR = 1.5-2.5). Basin models were used to integrate stratigraphic evidence with other data, in specific fission-track analysis of apatite and biomarker maturity, and indicate that maximum temperature (*ca.* 85°C) was attained during the first, Cretaceous burial event, while maximum depth (*ca.* 1 700 m below surface) and therefore maximum compaction was reached during the much shorter Miocene event (*ca.* 10 Ma b.p.). The two events were separated by an uplift phase where *ca.* 600 m of the overlying sedimentary rocks were eroded. Since maximum burial, the region of interest has been (and still is) uplifting at an average rate of 0.1 mm/a.
Boom Clay at Mol	Very detailed information exists on the entire Cenozoic stratigraphic column thanks to a series of boreholes. The precision of the parameters obtained along the stratigraphic column is in the order of decimetres. This allows reconstituting burial history with high precision (sequential stratigraphy). In the geological past, the Boom Clay at Mol appears to never have been deeper in the geological past than at the present day, in contrast to the Antwerpen region (Van Keer & de Craen, 2001). However, from a geomechanical point of view, *in situ* measurements show that the Boom Clay at Mol is over-consolidated. At present no explanation for this phenomenon exists (see also FEP 58).

Formation/ site	Results and conclusions
Boda Clay Formation at Mecsek	After the deposition of the Boda Clay Formation, sedimentation and subsidence continued to the Early Jurassic, resulting in an overburden of 3 500-5 000 m. During the Jurassic, the sedimentary facies changed from shallow-water to pelagic, but the thickness of the sediments was only some hundreds of metres. Uplift started in the Cretaceous, and there is no record of younger sediments. In summary, the maximum burial of the Boda Clay Formation is estimated at 4 000-5 000 m on the basis of stratigraphic evidence. On the basis of illite and chlorite crystallinity and of vitrinite reflectance, maximum temperature experienced by the formation is estimated at 200-250°C. K/Ar ages of illite (fraction <2 µm) yield 197 ± 10 Ma (Early Jurassic), which is interpreted as the date of maximum burial.
Pierre Shale in south Dakota	Geologic reconstructions of central South Dakota based on erosional remnants and sedimentological considerations indicate that *ca.* 400 m of overburden sediment has been eroded at the Hayes site in a series of lateral river erosion episodes (Neuzil 1993). Prior maximum overburden on the Pierre Shale at Hayes (South Dakota) was estimated from consolidation tests on cores using Casagrande method. This approach suggested as much as one km or more of overburden was eroded from the site (Neuzil, 1993).

50.3 Scaling issues

Burial and uplift are processes that occur on the scale of the sedimentary basin, i.e. on a regional scale. Samples on which burial and temperature histories are investigated typically come from boreholes. In most examples studied here, the results can be inter- or extrapolated to a larger area (mostly >10 km away from the investigation site) because lateral changes of the thickness of the overlying sediments or amounts of erosion do not change dramatically over such distances. Major differential vertical movements during burial and uplift would be expected to occur along regional faults, whose existence and position would be identified by regional field investigations (field mapping, seismics).

50.4 Scientific level of understanding

A substantial number of independent methods exist to constrain burial and temperature history. If these are used in combination, even complex geologic evolutions, such as in Opalinus Clay (two-stage burial and uplift, erosional gaps), can be reasonably well constrained and result in good system understanding. The important point is not to use individual methods in isolation but to integrate them, e.g. in basin models. Such models couple the burial and temperature histories and also provide a consistency check of the methods applied.

50.5 Linked FEPs

FEP 5	Hydraulic potentials and gradients in the host rock, including boundary conditions
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 53	Past deformation events

50.6 Level of understanding from a PA perspective and treatment in PA

Burial and temperature history play a role in different aspects of PA:

- The knowledge of burial or uplift rates over long time scales (e.g. several Ma) can be extrapolated into the future and be used e.g. for erosion scenarios. It can also be compared to vertical movements derived from levelling data spanning time scales of years to decades.
- Maximum burial depth is needed to calculate important geomechanical parameters, such as the over-consolidation ratio, some of which are useful in rock-mechanical conceptual models.
- Effects experienced by the formation during its natural evolution can be compared quantitatively with expected repository-derived effects. For example, the thermal pulse derived from high-level waste can be put into perspective by comparison with the maximum temperature during burial, and this facilitates the estimation of possible consequences of the thermal pulse.
- In many cases, data and evidence from occurrences of the host formation outside the target area are used in a performance assessment (e.g. data from Mont Terri are used in the Swiss PA for Opalinus Clay in the Zürcher Weinland). Burial history needs to be known over the whole region, in order to build a basis for the extrapolation of external data into the target area.

The methods to constrain burial history are manifold and well developed. Burial history is considered as relevant but also well understood in most cases.

50.7 Available reviews

None reported.

50.8 Planned work

None reported.

50.9 Overall evaluation

Burial history affects several PA-relevant parameters and conceptual models and is considered relevant. A substantial number of methods constraining basin evolution are available and lead, if applied in an integrative manner, to a good understanding.

51. PRESENT AND FUTURE GEOTHERMAL REGIME AND RELATED PROCESSES (FEP C1.2.1)

51.1 Definition and generalities

The geothermal regime is determined by the natural flux of heat from deep crustal and mantle rock to the surface. The surface temperature is established by local climatic conditions. The thermal gradient depends predominantly on the surface temperature, the geothermal heat flux and the thermal conductivity of the rock column. Locally, thermal gradients can be perturbed by advective heat transfer in flowing ground water. Within argillaceous formations, only heat transfer by conduction (diffusion) is to be expected. This FEP is relevant to the far field in connection with site characterisation and boundary conditions for affected-field processes.

51.2 Site-specific experimental information

Site-specific geothermal gradients can be determined by temperature measurements in boreholes. The thermal conductivity and capacity values for specific formations are based on laboratory and field measurements. Values for representative formations are given in FEP 32.

51.3 Scaling issues

None reported. Geothermal gradient measurements are on the local scale. Scaling problems with thermal rock properties are discussed in FEP 32.

51.4 Scientific level of understanding

The principles of heat transfer in natural material are well understood. Mathematical modelling tools for describing temperature regimes and their changes in response to changing thermal conditions are widely available.

51.5 Linked FEPs

FEP 32	Thermal rock properties
FEP 50	Past burial history

51.6 Level of understanding from a PA perspective and treatment in PA

Consideration of the geothermal regime is more likely to be an aspect of scenario analysis than part of a comprehensive PA model. Substantial changes in the geothermal regime, e.g. by the intrusion of a heat source (igneous sill or dike) at depth, are not expected over the time scales in the order of 1 Ma, so this FEP is not of prime importance.

Andra and SCK•CEN have modelled the geothermal regime under climatic conditions that would promote permafrost formation. This modelling indicates that the depth of the 0ºC isotherm would reach 300 m at Andra's Bure site but would not reach the depth of the Boom Clay at Mol.

51.7 Available reviews

Textbooks on geothermal systems or on the transport of heat and other substances in natural systems provide a background which is sufficient for the description and modelling of the geothermal regime.

51.8 Planned work

None reported.

51.9 Overall evaluation

In assessing the performance of an argillaceous site, it may be important to consider changes in the thermal regime if scenario analysis indicates the site could be subjected to changing thermal boundary conditions such as volcanic intrusions or serious changes in climatic conditions at the surface.

52. FUTURE CHANGES IN HYDROCHEMISTRY OF THE HOST ROCK AND OF SURROUNDING FORMATIONS (E.G. DUE TO OUT-DIFFUSION, WATER-ROCK INTERACTIONS, UPLIFT) (FEP C1.2.2)

52.1 Definition and generalities

This FEP refers to the changes in fluid chemistry due to the following effects:

- Uplift during the long-term evolution could bring about erosion of overlying strata exposing the host rock and surrounding units to new sources and types of recharge, or could open new discharge points easing the flow of water through the host rock or adjacent formations. Changing recharge could be of different chemistry, and increased water flow could bring about chemical changes by facilitating redox and other water-rock reactions.
- Diagenetic processes affecting the long-term evolution of the site region include the intrusion of saline or oxidising waters which could establish new boundary conditions for chemical reactions, flow and diffusion within the host rock and the repository environment. Such changes should be explored for possible inclusion in scenarios considered for PA.

52.2 Site-specific experimental information

Formation/site	Results and conclusions	References
Opalinus Clay at Mont Terri	The effect of uplift on the chemistry of pore-water is known. It is discussed in detail in FEPs 23-25.	Pearson *et al.* (2003)
Opalinus Clay in the Zürcher Weinland	Solutes not controlled by water-rock interaction, such as Cl, Br and SO_4, will diffuse out of the Opalinus Clay, thereby reducing overall salinity. This process has been initiated *ca.* 2-2.5 Ma ago by the infiltration of low-salinity water into the local Keuper aquifer and is currently ongoing. The reduction of Cl content is accompanied by a corresponding reduction of Na content. Over a time period of 1 Ma, the reduction of salinity will be <10%.	Nagra (2002)
Boom Clay at Mol	The last significant change was seawater transgression some 1.6 Ma ago. Since that time, the Campine Basin has evolved from a marine to a continental environment, and fresh water started to infiltrate into the aquifers surrounding the Boom Clay. At present, the average Cl concentration in the Boom Clay at Mol is as low as 28 mg/l.	

52.3 Scaling issues

Interpretation of water chemical changes is on the scale of the formation, thus suited for PA purposes. However, the available data base often refer to much shorter periods of time.

52.4 Scientific level of understanding

The chemical composition of pore-water in argillaceous formations is affected by the temporal evolution of ground waters in the embedding aquifers. In many cases, the past evolution of the ground waters can be used for extrapolations into the future. At least in the case of diffusion-dominated argillaceous formations, exchange rates will be slow and can often be predicted with confidence. For the Opalinus Clay, a well supported quantitative model is available.

52.5 Linked FEPs

FEP 7	Units over- and underlying the host formation: local and regional hydrogeologic framework
FEP 8	Diffusivity
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 18	Dissolution / precipitation of solid phases
FEP 20	Ion exchange
FEP 22	Thermodynamic and kinetic modelling data
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 25	Water residence times in the host formation
FEP 27	Redox buffering capacity of the host rock
FEP 50	Past burial history
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events

52.6 Level of understanding from a PA perspective and treatment in PA

As long as diffusion remains the dominant transport mechanism, this FEP is well understood quantitatively and of little relevance. The chemical changes due to diffusion are slow enough to be neglected over PA-relevant time scales. Existing uncertainties with respect to the chemical evolution of the embedding aquifers (e.g. salt water intrusion) can be covered by alternative scenarios in PA.

In fractured, advection-dominated systems, the chemical interaction between aquifers and host formation my be more rapid and spatially more heterogeneous. A good understanding of the flow system is required.

52.7 Available reviews

None reported.

52.8 Planned work

None reported.

52.9 Overall evaluation

This FEP will have minimal effect on repository performance even over long time scales provided diffusion remains the dominant transport mechanism between the argillaceous unit and adjacent formations. Should fracture flow be an important transport mechanism, the effects would be more rapid.

53. PAST DEFORMATION EVENTS (FEP C2.1)

53.1 Definition and generalities

Non-elastic deformations and the associated formation of natural fractures occurred in response to vertical movements in the sedimentary basin (burial, inversion) and/or to regional tectonic stresses (see also FEPs 2 and 3). Purely extensional structures (joints) are not very frequent in argillaceous media, except in highly indurated formations and in near-surface environments. By far the most relevant large-scale structures are faults, i.e. normal faults, thrusts and strike-slip faults.

While faults may not be active migration pathways over geological periods of time, fluid-flow events may occur during active faulting. Different deformation events may reactivate already existing structures, resulting in recurrent phases of fluid flow along faults. While these findings are well established in more permeable rocks, such as crystalline basement or sandstone, the importance of episodic flow along faults in argillaceous formations is not entirely clear, however most likely quite limited (FEP 54).

53.2 Site-specific experimental information

The occurrence and geometry of faults on a wide range of scales is described in FEPs 2 and 3. Among the formations considered here, those which did not experience major burial and inversion and therefore are weakly indurated (Boom Clay and Spanish Reference Clay) show only a low density of faults and fractures. On the other hand, highly indurated (i.e. deeply buried) formations, such as the Boda Clay Formation and the Palfris Formation at Wellenberg, are highly faulted and contain fracture networks of different origins and ages.

In the sedimentary basin of northern Switzerland, seismic evidence indicates that several deformation events occurred during the Mesozoic, and this is evident from the fact that the density of structures decreases with age (Birkhäuser *et al.*, 2001). For example, the top of the Opalinus Clay shows less features than its base, which argues for synsedimentary tectonics. The tectonic and neotectonic situation is addressed in Müller *et al.* (2002).

Fluid flow related to faulting can be recorded by fracture infills and/or wall-rock alterations along fractures. In the weakly indurated formations that were considered (Boom Clay, Spanish Reference Clay, Callovo-Oxfordian at Bure, Opalinus Clay), fracture mineralisations and veins are absent or very scarce. Their absence is taken as evidence of the lack of major fluid flow along fractures during and after faulting. In the Toarcian-Domerian at Tournemire, geodic calcite veins occur in dilatant parts of faults (Boisson *et al.*, 1998). In the Boda Clay Formation and in the Palfris Formation at Wellenberg, fracture infills are abundant and mostly related to events that occurred during deep burial of the formations. At Wellenberg, vein infills can be explained by local (m-scale) mass redistribution due to pressure solution and re-precipitation in pressure shadows (Mazurek, 1999).

53.3 Scaling issues

Natural non-elastic deformations result in structures on a wide range of scales, and different investigation methods provide data on different scales (see FEP 3 for details). The temporal scales over which the information relates are comparable, often even much longer than those required for PA predictions.

53.4 Scientific level of understanding

The understanding of geometric aspects of deformation events that occurred in the geological past is generally very good, with the exception of steeply dipping structures at sites where only vertical boreholes are available. On the other hand, in many cases it is difficult to date the deformation events. Events of fluid flow related to deformation events can be reconstructed on the basis of fracture mineralogy and geochemistry. The absence of mineralogical and geochemical evidence for fluid-flow events is a necessary but not sufficient argument for the extrapolation of the present-day situation to the future.

Formations that were deeply buried (several km) are often fractured, faulted and contain abundant veins and fracture infills. In most cases, faulting and mineralisation occurred at depth, at pressure-temperature conditions that are substantially different from present-day conditions and conditions expected for the future. Care must be taken to use only those features and processes observed in the rocks for extrapolations that are relevant for the physico-chemical conditions expected over PA-relevant time scales.

53.5 Linked FEPs

FEP 2	Size and geometry of the host rock and of surrounding units, migration path length
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 37	Geomechanical rock properties
FEP 50	Past burial history

53.6 Level of understanding from a PA perspective and treatment in PA

Knowledge of past non-elastic deformation events contributes to general system understanding, which is needed for the prediction of such deformations that may occur in future. While the deformation events themselves are of limited PA relevance, possible fluid-flow events associated to these deformations may be included in alternative PA scenarios of long-term evolution (FEP 54).

The attractiveness in studying past deformations lies in the fact that geological deformation structures occurring in the rocks today reflect the integrated history of the formation over geological time scales. Even if no major active deformation takes place at the present time (as evidenced e.g. by neotectonic surveys), evidence of past faulting events can be integrated in scenario development for PA.

53.7 Available reviews

None reported.

53.8 Planned work

None reported.

53.9 Overall evaluation

Faults and fractures in the rocks record the integrated effects of deformations over geological time scales. Deformations that can be expected in the future can be constrained by studying the evolution in the past.

54. FUTURE FAULT (RE)ACTIVATION, CHANGES IN MIGRATION PATHWAYS; CHANGES OF HYDRAULIC PARAMETERS; FLOW EVENTS (FEP C2.2)

54.1 Definition and generalities

In a dynamic natural system, stresses accumulate over long periods of time and may be instantaneously released in earthquakes. Such events of fault movement may change migration pathways, permeabilities, head distributions and thus result in flow events.

54.2 Site-specific experimental information

Formation/ site	Results and conclusions
Paris Basin (including the Callovo-Oxfordian at Bure)	The effects of permafrost on the hydrogeological evolution (mainly head distribution) have been studied by means of numerical simulations. The results indicate that the effects may not be completely irrelevant (slight increase of I doses; possibly less dilution in aquifers).
Opalinus Clay in northern Switzerland	In spite of the presence of major faults in Opalinus Clay, these are not associated with mineralisations and alterations and thus do not show any evidence of fluid-flow events related to faulting. Profiles of tracers in pore-water in the Benken borehole and at Mont Terri can be explained by diffusion and do not record any relationship to faults. Fluid flow related to seismicity in Opalinus Clay is discussed in Hicks (2002).
Boom Clay in NE Belgium	Active faults can be traced on the surface as escarpments. In NE Belgium, several active faults belonging to the Roer Valley Graben were studied by means of direct observation in trenches, by several geophysical methods (electrical tomography, high-resolution reflection seismics, boreholes) and by the study of the seismic activity. Studies of recent earthquakes give information about the depth of the movement and the displacement that took place (Ahorner, 1992).
Boda Clay Formation at Mecsek	Regional uplift is slow, and the generation of new faults is not expected in the next 1 Ma. However, a compressive regime has persisted over millions of years, witnessed by folding and thrusting of Pliocene sediments along existing (i.e. reactivated) faults. Fault (re)activation in the future is expected mainly along the margin of the Mecsek Mountains.
Mizunami Group at Tono	The steeply dipping Tsukiyoshi fault indicates 30 m of reverse movement and is observed to cut early to middle Miocene sediments interbedding with the several shale layers in the Tono mine. The fault is estimated to have been most active in the period 15 to 5 Ma (Koide *et al.*, 1996).

A geodynamic measuring station in the Mecsek region (Hungary) was in operation between 1991-1999 in the tunnel system at 1 000 m depth, but no activity was identified. According to nationwide seismological investigations, the following distribution of future earthquakes is expected:

time period, y	likelihood = 30%	likelihood = 10%	likelihood = 5%
100	5.5	6.0	6.3
500	6.2	6.6	6.8
1 000	6.4	6.8	7.1
10 000	7.2	7.6	7.9

The numbers indicate maximum earthquake intensities expected within the given time period with a given likelihood.

54.3 Scaling issues

Observations and measurements of fault movements generally relate to scales of hundreds of metres or more, which is in line with the scale required in PA (consideration of flowpath length). Major upscaling is needed in time, i.e. when recent or neotectonic movements are extrapolated into the future.

Water-rock interactions along faults record the integrated history of fluid-flow events over the lifetime of the fault, and thus refer to very long time scales, often longer than those needed for PA.

54.4 Scientific level of understanding

There is a number of techniques to address this FEP, such as the study of past deformation, water-rock interaction and fluid-flow events (FEPs 24, 53), neotectonic studies or conceptual considerations.

Major faults may occur within kilometres from planned repository sites, and their positions are generally very well known. They can be adequately characterised by geophysical methods and surface exposures (e.g. by trenching). Seismic activity along these faults in the future is possible (if not likely), even though difficult to study due to the often short observation window that is available. However, in most cases indirect evidence exists that the hydraulic significance of the faults has been negligible in the geological past, irrespective of their possible seismic activity. At the sites considered, there are no examples of faults through argillaceous host rocks where substantial water-rock interactions or changes of the hydrochemical environment were identified.

Hicks (2001) reviewed the conceptual models that explain fluid flow related to faulting (e.g. seismic pumps, suction pumps, fault valves). Field examples of all these mechanisms exist in the literature, but none of these has been shown to operate in low-permeability rocks such as argillaceous formations. Muir-Wood & King (1993) identified anomalous flow rates in rivers after seismic events and were able to explain these by stress redistribution along faults. However, these findings were made in higher-permeability formations, and their significance in argillaceous rocks has not been demonstrated. At a qualitative level, there is a basic level of scientific understanding regarding the hydrogeological consequences of fault (re)activation, but the scientific level of understanding at a more detailed, quantitative level is low.

54.5 Linked FEPs

FEP 3	Migration pathways, including heterogeneity and anatomy
FEP 7	Units over- and underlying the host formation: local and regional hydrogeologic framework
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 25	Water residence times in the host formation
FEP 37	Geomechanical rock properties
FEP 56	Future stress regime
FEP 57	Geomechanical effects of erosion/unloading

54.6 Level of understanding from a PA perspective and treatment in PA

In many PA studies, the (re)activation of faults, followed by transient or stationary fluid flow, is studied in *what if* scenarios. Except in highly indurated formations where fracture flow is importants, this FEP is considered as not very relevant and so is not treated in the base case of PA studies.

For the Boom Clay at Mol, the potential effect of a fault zone has been assessed in the PA study of Marivoet (1988). The assessment shows that the effect was not very relevant. Due to the creep of the Boom Clay, no open faults can be maintained but a zone with non-elastic deformation can be formed. Mechanical damage to the repository due to faulting can be excluded because the repository will be located outside of existing faults (such areas exist and can be explored).

54.7 Available reviews

Boom Clay: Demyttenaere (1988), Langenaeker (1998).

54.8 Planned work

Boom Clay at Mol: The digging of a trench is foreseen, in order to study the activity of the closest faults near to the site. The observations will take place during 2003, the studies finalised by early 2004.

Boda Clay Formation at Mecsek: Long-term leveling using the GPS measurement network is foreseen, consisting of 9 points and starting in 2000. A measurement was already done in 1998, on a network consisting of 8 points. A geodynamic measuring station consisting of a long extensometer was installed at 80 m depth in 2000 in an area where the Boda Clay Formation crops out, and was complemented by 3 short extensometers installed perpendicular to each other. The measurement series is planned for the long term and is done with continuous, automatic data recording. Its purpose is the characterisation of the three-dimensional deformation within the Western Mecsek Anticline.

54.9 Overall evaluation

The importance of this FEP is regarded to be relatively small because the positions of major faults are generally well known and there is no clear field evidence that faulting is related to major fluid-flow events in argillaceous rocks. In the Belgian assessment, even if a fault activation creates a fault that touches the repository, the fraction of radionuclides that can migrate through this fault is very small.

55. PRESENT-DAY STRESS REGIME (FEP C2.5)

55.1 Definition and generalities

The present-day stress regime is a basic attribute of the host rock and is intrinsically related to its geological and geomorphological setting. It constitutes an essential component in the repository system. As boundary condition it is an indispensable factor in the setup of a geomechanical model for the numerical analysis of the system.

Present-day *in situ* stress of the host rock is relevant predominantly for the following two reasons:

1. In the far field it is a controlling factor in the layout of the underground works. In the case, for instance, that the maximum horizontal *in situ* stress σ_H is greater than the vertical stress σ_v, the emplacement tunnels and galleries are optimally oriented if they are aligned in the direction of σ_H.

2. In the affected field it controls, amongst others, the shape and extent of the EDZ, the ground support required and the layout of the engineered barrier system.

The term "present-day stress regime" is generally understood as the state of stress which is currently acting in a geological formation without any man-induced disturbances. It is also termed "primary", "geologic", "virgin", "*in situ*" or "initial" state of stress.

In general terms, the 3-D state of stress at a point is specified by six components (three normal stress and three shear stress components). Alternatively, the state of stress may be described in terms of three principal stresses σ_1, σ_2 and σ_3, with σ_1 being termed the major, σ_2 the intermediate and σ_3 the minor principal stress ($\sigma_1 \geq \sigma_2 \geq \sigma_3$; compression positive). Each principal stress is defined by its magnitude and orientation (Brady and Brown, 1985). The orientation of the three principal stresses is normal to each other, i.e. the orientations constitute units which are not entirely independent of each other. Very common is the consideration of the normal stress components which are acting in vertical (σ_v) and in distinct horizontal directions (σ_H and σ_h with σ_H being the major and σ_h the minor horizontal normal stress component). Particularly, in connection with stress measuring tests in vertical boreholes based on hydraulic fracturing, it is (often tacitly) assumed that σ_v, σ_H and σ_h are principal stresses.

In an actual project situation it may be possible to roughly estimate the order of magnitude of the primary *in situ* principal stresses and their orientations from observations of so-called "stress indicators" and knowledge of the general morphological and geologic setting. However, the uncertainty of the actual values is substantial in the absence of direct measurements (Goodman, 1980). In rock engineering practice, the question of the present-day state of stress therefore is intrinsically connected with *in situ* stress measurements and with site-specific observations, e.g. of the breakout configurations in boreholes or in underground openings.

55.2 Site-specific experimental information

Formation/site/ reference	Experimental techniques employed	Results and conclusions
Toarcian-Domerian at Tournemire (Boisson *et al.*, 1998)	Hydraulic fracturing	Two campaigns have been performed but lead to difficulties in interpretation of the results. One important finding is the relevant influence of surface topography (the site is located in a E-W massif with major valleys in the north and south).
Spanish Reference Clay in a Tertiary basin (Enresa, 1999)	Tests (presumably hydraulic fracturing) performed in one vertical exploratory drillhole	The major horizontal stress σ_H has an azimuth of 125°. It is assumed that the principal stresses are oriented in horizontal and vertical directions. Magnitudes (for 230 m < z < 300 m depth range): $\sigma_H = 4.96 + 0.0104\ (z - 230)$ $\sigma_h = 4.16 + 0.004\ (z - 230)$ $\sigma_v = \rho\ g\ z$ where: σ_H; σ_h = major / minor horizontal stress [MPa] σ_v = vertical stress [MPa] (assumed) ρ = rock density [kg / m^3] g = gravity acceleration [m / s^2] z = overburden height [m].
Opalinus Clay at Mont Terri (Martin & Lanyon, 2002)	Under- and overcoring, borehole slotting, hydraulic fracturing and back-analysis from convergence behaviour of the underground research laboratory	$\sigma_1 \approx \sigma_v \approx 6.5$ MPa acting sub-vertically (gravity-dominated) $\sigma_H \approx \sigma_2 \approx 4.5$ MPa, sub-horizontally in SSE – NNW (155°) direction. $\sigma_h \approx \sigma_3 \approx 3.5$ MPa, sub-horizontally in ENE – WSW (65°) direction.
Opalinus Clay in the Zürcher Weinland (Nagra, 2001)	Hydraulic fracturing and borehole breakout analysis	σ_H oriented in SSE – NNW direction (170° ± 10°) and being a principal stress. Magnitudes (at about 650 m depth): $\sigma_H \approx 1.5\ \sigma_h$ ($\approx$ 22.6 MPa) $\sigma_h \approx \sigma_v = \sigma_3 \approx \sigma_2 = \rho\, g\, z = 15.1$ MPa. The direction of σ_H is consistent with that derived from stylolites, indicating that the stress regime has not drastically changed over several Ma.
Boom Clay at Mol	piezometers, self-boring pressiometer	Results referring to the underground research laboratory: lithostatic pressure σ_V (theoretical) = 4.6 MPa; σ_V (experimental) = 3.4 MPa; hydrostatic pressure σ_{aq} = 2.3 MPa; σ_h oriented NE-SW; $K_0 = \sigma_{h/} / \sigma_v = 0.9 - 1.2$. Reference: Li (*in prep.*) (CLIPEX experiment, final report).

Formation/site/ reference	Experimental techniques employed	Results and conclusions
Boda Clay Formation at Mecsek (Gerner *et al.*, 1999)	Short-term programme with the application of hydraulic fracturing, sleeve fracturing and overcoring.	No conclusive information from sleeve fracturing and overcoring. In the region of the underground research laboratory at a depth of 1 030-1 080 m, the highest stress component amounts to about 30 MPa. The σ_3/σ_1 ratio is between 0.6 and 0.9. Current experimental data suggest a quasi-isotropic compression stress field. This, however, is in contradiction with the World Stress Map which for the Transdanubian region indicates a dominant compression in NE-SW direction.
Mizunami Group at Tono (Maeda *et al.*, 1999) Kamaishi mine (crystalline rock; Matsui *et al.*, 1997)	Various methods, amongst them measurements on cores and acoustic emission. Study on the applicability of the existing stress measuring methods.	Generally: *In situ* stress conditions differ quite considerably in soft rock from those in hard crystalline rock. In the Tono area, the *in situ* stress state is not influenced by a major geological fault (Tsukiyoshi fault). The measured vertical stress component corresponds with the overburden pressure at any depth.
Pierre Shale in south Dakota (Neuzil, 1993)	Borehole methods (unspecified)	Essentially a lithostatic stress state with no deviatoric stresses.

55.3 Scaling issues

Stress is a physical quantity which, by definition, applies to a point. The mentioned stress measuring methods integrate point stresses over a domain of centimetres (e.g. for overcoring and borehole slotting), decimetres (borehole breakout analysis) and metres and beyond (hydraulic fracturing).

Upscaling from the stress measuring domain to the 100 m to 1 000 m range of a repository does not appear to be a principal problem. Problems may exist in providing enough financial and technical resources for carrying out a sufficiently large number of (relatively expensive) stress measurements that may be needed for the coverage of a larger domain, depending on the degree of homogeneity of the *in situ* stress field.

An integrated approach is essential for upscaling of the stress measurements. In such an approach, not only stress measuring results and large-scale geologic structures are to be considered, but also a thorough validation of the results has to be carried out by geomechanical and geophysical studies such as the back-analysis of the mechanical behaviour of underground research laboratories, systematic borehole breakout analyses and the application of fault plane solution techniques to nearby natural or man-made seismic events.

55.4 Scientific level of understanding

The global and regional present-day stress regimes are generally reasonably well understood as, for example, is evidenced in the World Stress Map. However, in the absence of site-specific stress measurements, the general level of understanding is insufficient with regard to the stress regimes acting at the local scale, including that of the usual scale of a repository system. The global stress state can be quite substantially superimposed by local factors, to a degree that the local stress state may have no resemblance with the global or regional states. Factors which are responsible for such stress variations are irregular morphology, residual stresses, stress inhomogeneities due to lithologic changes (different strata) and geological faults.

A number of methods and tools are available for site-specific measurements of the stress field. A major problem is the fact that in over-consolidated argillaceous formations, many of the standard stress measuring methods do not work properly either technically and/or from a conceptual point of view. In such formations, the borehole walls tend to be unstable. Thus it is often difficult, if not impossible, to provide regular, cylindrical boreholes which are required in most stress measuring tests (e.g. hydro fracturing, overcoring). Linearly behaving borehole wall rocks are also an intrinsic requirement for the applicability of most standard stress measuring methods such as overcoring and borehole slotting. Moreover, disturbances and fracturing of the borehole wall material are common. Another problem which is notorious in argillaceous materials is the effect of material and rock mass anisotropy onto the state of the *in situ* stresses as well as onto the stress measuring results.

Careful drilling in combination with purpose-designed, -executed and -evaluated tests are required to alleviate these problems. The use of independent methods in parallel adds confidence to the experimental results.

55.5 Linked FEPs

FEP 5	Hydraulic potentials and gradients in the host rock, including boundary conditions
FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 37	Geomechanical rock properties
FEP 50	Past burial history

55.6 Level of understanding from a PA perspective and treatment in PA

Knowledge of the present-day *in situ* stress regime of the host-rock formation is a prime requirement for repository design and construction. Conceptually and technically, it is feasible to gain such knowledge, provided that the geological structure is not too complex, sufficient funding is available for a reasonably large number of *in situ* stress measurements and an integrated approach is chosen in the evaluation of stress data. In most sites considered it is felt that such knowledge is not yet available to the degree needed. The Zürcher Weinland in NE Switzerland is an exception: The regional *in situ* stresses have been determined to a level of accuracy which is believed to be sufficient for the actual stage of the project development.

Within a siting study, the present-day *in situ* stress regime is an essential element of the geological boundary conditions, and its explicit specification is required. The geologic state of stress has implications in both the far and the affected field of a repository. In the far field, the geologic stresses have to be considered in the design of the layout of underground works such as the optimisation of the orientation of tunnels and galleries with regard to the orientation of the principal *in situ* stresses. In the affected field, the stress regime is a controlling factor for the shape of underground openings, the shape and extent of the EDZ, the ground support system and the layout of the engineered barrier system.

55.7 Available reviews

None reported.

55.8 Planned work

Formation/site	Planned activities
Toarcian-Domerian at Tournemire	Possible new attempts with alternative techniques (borehole slotting; new type of hydrofracturing) in addition to analysis of structural stress indicators. No clear plans at the moment.
Boda Clay Formation at Mecsek	Precise deformation measurements (strain ellipsoid) in a sub-surface geodynamic measuring station by permanently installed extensometers in combination with electronic liquid-level inclinometers. At the surface: Series of long-term GPS measurements.

55.9 Overall evaluation

The present-day stress regime is a result of the current site-specific morphological and structural conditions in combination with the geologic history of the host rock. It is an important FEP in support of repository design, construction and site characterisation. Within a siting study, it is an essential element in the specification of the boundary conditions.

For the specification of the present-day stress regime, an integrated approach is required with includes the identification and assessment of “stress indicators” (e.g. borehole breakouts), consideration of the general morphological and geologic setting, back analyses of large-scale experiments (e.g. in underground research laboratories) and carrying out of *in situ* stress measurements. Against the background of the specific technical and conceptual problems in argillaceous formations, the stress measurements have to be purpose-designed. Common practice is to employ various stress measuring methods for comparison.

56. FUTURE STRESS REGIME (FEP C2.6)

56.1 Definition and generalities

This FEP relates to the future geological and geomorphological setting of the host rock over PA-relevant geological times. It is intrinsically related to the geodynamic development of the host rock formation in connection with pertinent geological processes such as uplift, erosion, subsidence, sedimentation and tectonic stress regimes.

56.2 Site-specific experimental information

The direction of present-day σ_H in Opalinus Clay in the Benken borehole is consistent with the one derived from stylolites, indicating that the stress regime has not drastically changed over the past several Ma. This is taken as evidence that the regional tectonic stress field will remain constant at least over the coming 1 Ma. However, due to the effects of ongoing uplift (0.1 mm/a), σ_v will decrease. Within 1 Ma, maximum erosion is 200 m, reducing the overburden of the repository from 650 to 450 m. The related decrease of the horizontal stress components depends on the model/concept chosen (Nagra, 2002).

56.3 Scaling issues

None reported.

56.4 Scientific level of understanding

Over the time scales considered here, major changes of horizontal stresses due to a changing geodynamic situation are not likely. However, vertical movements may be relevant.

Regional uplift in combination with erosion will lead to a decrease of the magnitudes of the relevant stress components σ_H, σ_h and σ_v of the host rock (for definition of σ_H, σ_h and σ_v see FEP 55). The magnitudes of the decrease of these stress components will be unequal. The stress release will be greatest in the vertical direction and smallest in horizontal directions (due to the continuous confinement). This has the consequence that the proportion between horizontal and vertical stresses σ_H/σ_v will be increased. The orientations of the principal stresses tend to reverse in the sense that, for instance, a vertically oriented σ_1 is turned into a horizontal direction and *vice versa* for σ_2 and/or σ_3 (Bock 1975). With continued uplift and erosion, the growing stress anisotropy may be released by inelastic processes (e.g. by the formation of surface-parallel extension fractures). Based on field evidence from several argillaceous formations, this typically happens in the uppermost decametres below surface.

In the case of subsidence in combination with sedimentation, the higher overburden pressure will lead towards higher values of the total stresses, whilst the ratio the horizontal to the vertical stress components will tend towards unity ($\sigma_H/\sigma_v \rightarrow 1$; isotropic stress state). This would generally mean more favourable boundary stress conditions for the repository. If the subsidence rate is high and the hydraulic conductivity of the host rock is comparatively low (the latter condition tends to prevail in argillaceous formations), significant pore-water excess pressures may develop, particularly if the overburden pressure σ_v exceeds the pre-consolidation pressure (i.e. the maximal pressure of the geological past). This, in turn, leads to the situation that the effective stresses are not increased to the degree as is the case for the total stresses (see FEP 58).

56.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 37	Geomechanical rock properties
FEP 50	Past burial history
FEP 55	Present-day stress regime
FEP 57	Geomechanical effects of erosion / unloading
FEP 58	Consolidation due to burial
FEP 59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)

56.6 Level of understanding from a PA perspective and treatment in PA

Knowledge of the future *in situ* stress regime is required as an explicit boundary condition if the long-term evolution is modelled within the domain of the repository. The future *in situ* stress regime is intrinsically related to the geodynamic and morphological development of the host-rock formation (uplift, erosion, subsidence, sedimentation, tectonic stress; see FEPs 57-59).

It is generally recognised that the regional tectonic stress regime at any of the sites considered will not change substantially over PA-relevant time scales. However, the stress field at repository level may change in response to possible changes of lithostatic pressure due to erosion or sedimentation (see also FEP 57). In spite of the uncertainties related to the evolution of horizontal stresses in response to a changed vertical stress, knowledge is regarded as sufficient for PA purposes.

56.7 Available reviews

None reported.

56.8 Planned work

None reported.

56.9 Overall evaluation

The regional tectonic stress regime is not expected to change substantially over PA-relevant time scales. However, the stress field at repository level may change in response to possible changes of lithostatic pressure due to erosion or sedimentation. In specific, the possibility of inelastic deformation due to erosion merits consideration in PA.

57. GEOMECHANICAL EFFECTS OF EROSION/UNLOADING (FEP C3.1)

57.1 Definition and generalities

Within this FEP, the term “erosion” is understood in the sense of *vertical erosion,* which is the natural removal of overburden strata by the action of rivers, wind, glaciers or marine erosion. Vertical erosion is commonly the consequence of regional uplift. A special form of vertical erosion is the melting of glaciers.

Vertical erosion results in a partial or complete unloading of the underlying strata. As a consequence, the magnitudes of the total *in situ* stresses acting within these strata are reduced. This applies in particular to the magnitude of the vertical normal stress component σ_v. The evolution of the horizontal stresses is less clear and is addressed in FEP 56. Uplift and vertical erosion are commonly associated with a significant reduction of pore-water pressures in the near-surface strata, e.g. due to the formation of surface-parallel extensional fractures. The pore-water pressure may be reduced to a degree that significant underpressures (suction) may develop.

The erosion rates vary in space (e.g. topography, presence and number of valleys) and time (e.g. geodynamic processes, climatic cycles, change of the erosion base level). Erosion can be verified either indirectly by geologic and geomorphological evidence or directly by geodetic measurements.

57.2 Site-specific experimental information

Formation/site/ reference	Investigation techniques employed	Results and conclusions
Opalinus Clay in the Zürcher Weinland (Nagra, 2002)	• Basin modelling based on a large number of data pertinent to burial history • Study of vertical movements during the Quaternary, incl. erosion patterns • Geodetic levelling • Conceptual considerations of the geomechanical response to stress release • Observations in Opalinus Clay situated at different depth levels	An uplift rate of 0.1 mm/a was consistently derived from several methods. Within the time scale of 1 Ma, stress release in the repository will be limited and will not lead to inelastic deformations. An extensive data base from Opalinus Clay at different depth levels is available. It shows that existing fractures are not hydraulically active if the local overburden exceeds 200 m. It is concluded that pre-existing fractures remain sealed during uplift until they reach the depth level of 200 m, where some (but by far not all) may become transmissive. Hydraulic overpressures observed today will be dissipated in future, but this process is difficult to quantify.

Formation/site/ reference	Investigation techniques employed	Results and conclusions
Boda Clay Formation at Mecsek (Ronai, 1974, Pecsi *et al.*, 1984)	Conventional geodetic levelling. Geological and morphological evidence	Uplift rates are ~ 0.5 mm/a.
Pierre Shale in south Dakota (Neuzil, 1993)	Hydraulic tests in boreholes, long-term monitoring	Observed underpressures are interpreted as a consequence of erosional unloading.
Canadian argillaceous formations	Evaluation of petrophysical data	Uplift could result in the development of sub-hydrostatic pressures caused by increased porosity.

57.3 Scaling issues

If different methods are applied to estimate uplift and erosion rates (e.g. basin modelling, Quaternary geomorphology, geodesy), a wide range of time scales is covered, so scaling in time is not an issue. Spatial scaling involves the possible role of major faults that may separate blocks with different uplift rates. Such faults are generally well known from regional investigations.

57.4 Scientific level of understanding

The currently available methods are considered to be adequate to allow for a sufficiently accurate delineation of this FEP. The consequences of the reduction of vertical stress on the overall mechanical behaviour of the formation can be reasonably well established by means of conceptual considerations.

57.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 37	Geomechanical rock properties
FEP 41	Swelling
FEP 50	Past burial history
FEP 56	Future stress regime
FEP 59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)

57.6 Level of understanding from a PA perspective and treatment in PA

A good database is required to constrain the possible erosion rates over PA-relevant time scales. Conceptual considerations on inelastic deformations in response to stress release are considered to be sufficient for PA purposes. Such deformations typically occur at very shallow levels, so will come into play only shortly before exhumation of the repository.

57.7 Available reviews

None reported.

57.8 Planned work

Formation/site	Planned activities
Bresse region (France)	Acquisition of the geological parameters which are required to quantify erosion: Field surveys (specific mapping, age dating) and modelling of the incision of rivers in 4D (i.e. space and time).
Boda Clay Formation at Mecsek	Long-term annual GPS measurements in combination with deformation measurements in the geodynamic measuring station.

57.9 Overall evaluation

The geomechanical consequences of erosion process are subject to ongoing studies, however the principal features seem to be well understood. Evidence from the Opalinus Clay suggests that the PA-related hydro-mechanical effects of erosion remain minor, as long as the overburden of the repository remains higher than about 200 m.

58. CONSOLIDATION DUE TO BURIAL (FEP C3.2)

58.1 Definition and generalities

The title of this FEP can be understood in different ways.

In a general sense, consolidation is a time-dependent transfer of a water-saturated cohesive soil or silty-argillaceous rock into a higher-density state (reduction of porosity) due to increased overburden pressure. The transfer is controlled by the rate at which the excess pore-water pressure is dissipated (expulsion of pore-water). The dissipation process is a function of the hydraulic conductivity of the soil or rock, the drainage conditions and the loading rate.

In a narrow sense, consolidation is understood as a compaction process of the EDZ due to swelling of the host rock or of the backfill. A major part of this process will take place in unsaturated conditions. The term “consolidation” therefore seems to be less appropriate and may be substituted by the term “compaction”, “re-compaction”, “homogenisation” or similar.

Within the context of this FEP, consolidation is understood in the general sense. It is a process that may become effective when the repository host rock will be subject to subsidence in combination with sedimentation. Considering the fundamental geomechanical stress equation as formulated by Terzaghi (1925)

$$\overline{\sigma}_{tot} = \sigma' + p$$

with: $\overline{\sigma}_{tot}$ = total stress
σ' = effective stress
p = pore-water pressure,

three scenarios are principally possible with regard to the pore-water pressure development when a rock formation is subjected to an additional overburden pressure due to burial:

1. Saturated conditions and high hydraulic conductivity: The pore-water pressure remains hydrostatic (equivalent to the hydraulic head).
2. Saturated conditions and low hydraulic conductivity: Excess pore-water pressure develops (pore-water cannot be expelled at the rate at which the overburden pressure is increased).
3. Underpressured conditions and low hydraulic conductivity: In the case of basin inversion, a buried formation will be uplifted and decompacted, leading to over-consolidation and to the development of underpressures. In certain cases, this could also lead to the exsolution of gas and thus to unsaturated conditions. Re-loading by increased overburden yields a predominantly elastic response of the rock as long as the maximum overburden pressure of the geological past is not exceeded. No excess pore-water pressure will develop, and there will be no consolidation process at all.

58.2 Site-specific experimental information

Formation/site/ reference	Investigation techniques employed	Results and conclusions
Opalinus Clay in the Zürcher Weinland (Nagra, 2002)	Basin evolution study Geophysical-geotechnical logging of the Benken borehole in conjunction with review of data from petroleum exploration wells	Opalinus Clay was subjected to two successive stages of burial and consolidation (FEP 50). Maximum burial and consolidation in the Zürcher Weinland occurred before *ca.* 10 Ma, and the area has been uplifting since at an average rate of 0.1 mm/a. Slow uplift and unloading will occur during future long-term evolution, so further consolidation is not an issue for PA. In a regional study, a good correlation was found between maximum burial depth of the Opalinus Clay and porosity.
Boom Clay at Mol (Horseman *et al.*, 1987, Li *in prep.*)	Piezometers and self-boring pressiometer	Resulting over-consolidation ratio of 2.4 but no geological evidence of deeper burial than present state.
Boda Clay Formation / NE margin of the Drava Basin; W-part of the Szentlorinc-Pecs Basin (Ronai, 1974)	Conventional geodetic levelling Geological evidence	Subsidence rates of ~ 0.5 mm/a.

58.3 Scaling issues

See FEP 57.

58.4 Scientific level of understanding

It is generally felt that this FEP is reasonably well understood. This, in particular, applies to the Opalinus Clay of the Zürcher Weinland where a comprehensive model of the basin evolution and the geomechanical implications has been developed. The consistency of measured permeability / porosity values with the basin / palaeo-pressure history is an aspect that needs further consideration.

58.5 Linked FEPs

FEP 14	Lithology, mineralogy of rocks and fracture infills
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 33	Thermally induced consolidation of the host rock
FEP 37	Geomechanical rock properties
FEP 50	Past burial history

FEP 51	Present and future geothermal regime and related processes
FEP 56	Future stress regime
FEP 59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)

58.6 Level of understanding from a PA perspective and treatment in PA

Consolidation may have the following consequences that are relevant to PA:

1. Anomalous pressures (overpressures) may be generated (see FEP 59).
2. The hydrogeological properties of the argillaceous host rock may change (in particular the permeability, the porosity and the diffusivity).
3. The geomechanical properties may change (strength and plasticity).

In principle, the PA results are sensitive to all these aspects. However, none of the sites considered is being buried at rates sufficient to result in PA-relevant consequences over time scales in the order of 1 Ma. Therefore, while conceptual understanding is regarded as sufficient, no relevance is attributed to this FEP in PA studies.

58.7 Available reviews

None reported.

58.8 Planned work

Drava and Szentlorinc-Pecs basins (Hungary): Long-term annual GPS measurements in combination with deformation measurements in the geodynamic measuring station.

58.9 Overall evaluation

The geological and geomechanical features of the consolidation process are well understood. To increase the level of the confidence in the common hydrogeological and geomechanical models and data bases over PA time scales, a better understanding is desirable of how further consolidation would affect the hydrogeological and geomechanical properties of the host rock formation.

59. FUTURE EVOLUTION OF HYDRAULIC POTENTIALS AND GRADIENTS (E.G. DUE TO EROSION OR BURIAL) (FEP C3.3)

59.1 Definition and generalities

Geological processes such as sedimentation, erosion or glacial stages affect hydraulic potentials and gradients in a deep argillaceous formation. First, such processes may lead to major changes in the hydraulic conditions in the embedding, more highly permeable rock units. Because of the low hydraulic conductivity of argillaceous formations, the time required to equilibrate their hydraulic potentials can be very long (many thousands to millions of years). Second, a change in overburden may result in volumetric deformation within the argillaceous formation. Increasing the load can lead to further consolidation (FEP 58), while unloading can lead to an elastic rebound, swelling or even fracturing (FEP 57). By consequence, currently measured potentials may represent non-equilibrium conditions (see FEP 5).

59.2 Site-specific experimental information

Non-equilibrium (abnormal) hydraulic potentials have been measured in several argillaceous formations (see FEP 5). However, observation times are much too short compared to the long equilibration times of natural hydraulic disequilibria, so the rates of equilibration are difficult to constrain.

At several sites, geodetic measurements are performed to determine current rates of uplift or subsidence. Such measurements, together with data based on the long-term burial history (FEP 50), are used to predict future vertical movements and the evolution of topography. These factors also determine the future evolution of potentials in the aquifers and in the argillaceous formation itself.

59.3 Scaling issues

Because the geological, hydrogeological and geomechanical processes governing the future evolution of hydraulic potentials are very slow, the temporal extrapolation of current observations is particularly difficult. For the extrapolation of the occurrence of future glaciations, the Milankovitch astronomical theory is well established (Loutre & Berger, 2000) but could be affected by a strong impact of anthropogenic CO_2 release to the atmosphere.

59.4 Scientific level of understanding

The basic phenomena are well understood, and the hydro-mechanical models to explain over- or underpressures due to changes in hydraulic boundary conditions or load on an argillaceous formation are available. Similarly, the potential effects of glaciations (ice loading, permafrost) on hydraulic potentials and gradients are rather well understood. Palaeo-hydrogeological studies in combination with the Milankovitch astronomical theory have been used to predict future evolution of hydraulic potentials in sedimentary basins (e.g. Marivoet *et al.*, 2000). However, the site-specific understanding of the future evolution of geological processes such as uplift and subsidence, often remains poor.

59.5 Linked FEPs

FEP 5	Hydraulic potentials and gradients in the host rock, including boundary conditions
FEP 6	Hydraulic properties of the host rock
FEP 7	Units over- and underlying the host formation: local and regional hydrogeologic framework
FEP 23	Palaeo-hydrogeology of the host formation and of embedding units
FEP 24	Evolution of pore-fluid (water and gas) chemistry and mineralogy in the host formation and in embedding units
FEP 25	Water residence times in the host formation
FEP 50	Past burial history
FEP 54	Future fault (re)activation, changes in migration pathways; changes of hydraulic parameters; flow events
FEP 56	Future stress regime
FEP 58	Consolidation due to burial
FEP 59	Future evolution of hydraulic potentials and gradients (e.g. due to erosion or burial)

59.6 Level of understanding from a PA perspective and treatment in PA

Decreasing or increasing of the load on an argillaceous formation will lead to the development of over- or underpressures, and this can lead to a water flux out of the formation or into the formation. In case of underpressure in the host formation, the incoming water flux might hinder the transport of radionuclides out of the repository, while in case of overpressure it might lead to an enhanced outward radionuclide transport because the hydraulic gradient points out of the formation on both sides.

In diffusion-dominated formations, even an increase of the outward advective flux due to the relaxation of overpressure is likely to be of low relevance because the expected changes in gradients and resulting advective fluxes are generally not drastic enough to result in advection as the dominant transport process. On the other hand, in advection-dominated systems, advective flux will increase linearly to the increase of the hydraulic gradient and thus may lead to enhanced radionuclide transport.

Overpressures observed today in the Opalinus Clay of the Zürcher Weinland may at least partially be due to consolidation during maximum burial of the formation 10 Ma ago. Given the undisputedly long time scales related to the dissipation of the overpressures in this diffusion-dominated formation, these are unlikely to drive significant advective transport. Thus, they are neglected in the PA formulation of transport models for the geosphere. Better understanding of the underlying processes for the generation of overpressures would add further confidence.

The influence of the changes in hydraulic potentials induced by glaciations (changing loads, permafrost) on radionuclide transport have been explicitly treated in performance assessment studies for the Mol site and the Paris basin (Certes *et al.*, 1997). The effects of glacial loads on pore-water pressures in Opalinus Clay were also quantified, and the related fluxes are negligible according to model calculations (Nagra, 2002).

59.7 Available reviews

None reported.

59.8 Planned work

None reported.

59.9 Overall evaluation

This FEP is of importance for understanding the potential evolution of the whole hydrogeological system. At the considered sites, no important effects on the outcome of PA studies are expected, even though, it may have some importance in advection dominated systems. Current burial rates are typically too slow to result in significant consolidation and a major pore-pressure increase over a time scale of 1 Ma. Thus, for the considered formations, overpressures may be neglected in the formulation of transport models for the geosphere. The only exception is the possible influence of glaciations (changing loads, permafrost) in some but not all cases.

SECTION III

References

The numbers behind each reference refer to the FEP number
in Section II where this reference is quoted.
S.I = quoted from Section I.

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