

# Technical Report 15-04

Grimsel Test Site  
Investigation Phase VI

## **Main outcomes and review of the FEBEX In Situ Test (GTS) and Mock-up after 15 years of operation**

March 2016

G.W. Lanyon, I. Gaus

**National Cooperative  
for the Disposal of  
Radioactive Waste**

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This report was prepared by I. Gaus and G.W. Lanyon. It draws heavily on the reporting of the FEBEX I, II, NF-PRO and FEBEXe projects together with the many published papers concerning FEBEX. Data from the Mock-up and In Situ Test were kindly provided by AITEMIN and CIEMAT. Report contributions were made by M. Villar & P.L. Martín of CIEMAT (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas), A. Gens of UPC (Universitat Politècnica de Catalunya), J. García-Siñeriz & I. Bárcena of AITEMIN (Asociación para Investigación y el Desarrollo Industrial de los Recursos Naturales), and J. Samper & L. Montenegro of UDC (Universidade de La Coruña).

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## **Foreword**

### **The Grimsel Test Site**

Nagra and its partners have been conducting underground research at the Grimsel Test Site (GTS) since 1984. The projects have contributed substantially to the development and confirmation of safe geological disposal concepts and to the characterisation of potential host rock formations. The GTS is reached by an access tunnel belonging to the Kraftwerke Oberhasli AG (KWO), the local hydro-power company.

The tunnels of the GTS were excavated in 1983 and 1984 using both a tunnel boring machine (TBM) and drill and blast techniques. Expansion of the site in 1995 and 1998 provided space for two large-scale demonstration tests. The branching tunnel system of more than 1 km in length is located at an elevation of 1'730 m a.s.l., about 400 m beneath the Juchlistock, in the granite and granodiorite of the Aar Massif that was formed some 300 million years ago. As part of the characterisation studies, over 5 km of cored boreholes have been drilled so far. The local geology is ideal for the investigation of a wide range of experimental concepts and scientific issues with both tectonically overprinted and fractured areas as well as zones of homogeneous intact rock.

More than two dozen organisations and research institutes from twelve countries together with the European Union have participated in the six phases of the research programme. Each phase has focused on the key issues at the time, attempting to anticipate the next steps in national programmes for the long-term management of radioactive waste. The 15-year Phase VI began in 2003 and is dedicated to integrative projects with: a) field experiments under repository-relevant boundary conditions, i.e. large-scale, long-term experiments with realistic hydrogeological settings; and b) projects addressing the implementation of a geological repository in terms of engineering feasibility, potential construction impacts on the surrounding rock, operational aspects, closure, and monitoring. A radiation controlled zone of IAEA Level B/C allows field experiments to be carried out with radioactive tracers.

The GTS has emerged from its first three decades as an internationally renowned research laboratory in the field of safe disposal of radioactive waste in deep geological repositories. It has firmly established its roles as a strong driving force for scientific and technological progress, as an effective platform for international cooperation, as a hands-on training stage for knowledge transfer to the younger generation, and as a host for transparent dialogue with decision-makers and the public.

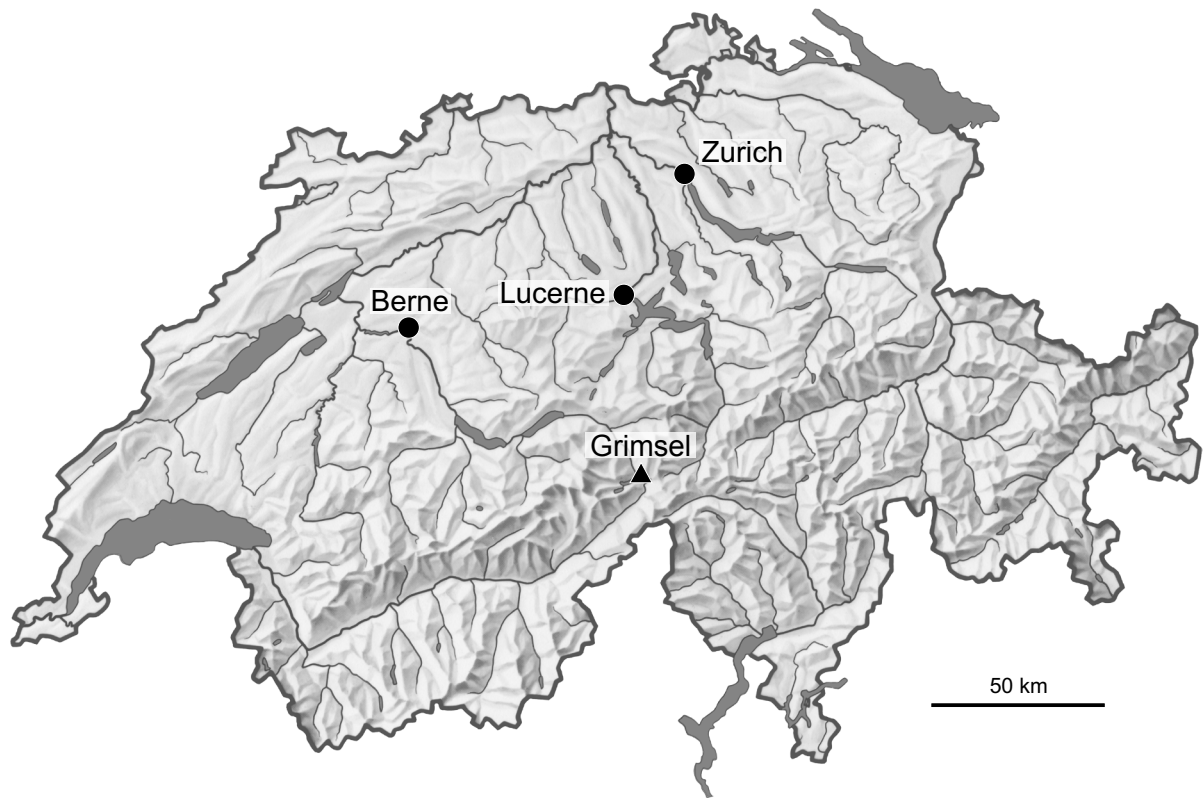
## **The FEBEX project**

The Full-Scale Engineered Barriers Experiment (FEBEX) was designed to demonstrate the feasibility of construction of the engineered barriers, and to increase the understanding of coupled processes in the near-field of a geological repository for high-level waste (HLW). FEBEX comprises a full-scale In Situ Test at the Grimsel Test Site, a large-scale Mock-up Test, a supporting laboratory test programme and modelling activities.

From inception in 1995 to the year 2015, FEBEX was operated under four different institutional frameworks. FEBEX I and II (1995 – 2004) focussed on demonstrating feasibility and verification of the performance of the engineered barriers, while the NF-PRO (2005 – 2007) and FEBEXe projects (2008 – 2014) focussed on development of detailed understanding of near-field processes and early-time coupled processes, respectively. Results from these four projects are summarised in this report. From 2015 onwards, FEBEX is continued as FEBEX-DP – the dismantling project.

Support has been provided as in-kind and financial contributions by the following past and present FEBEX project partners: AITEMIN (Asociación para Investigación y el Desarrollo Industrial de los Recursos Naturales, Spain), Andra (Agence Nationale pour la Gestion des Déchets Radioactifs, France), BGR (Federal Institute for Geosciences and Natural Resources, Germany), CIEMAT (Centro de Investigaciones Energéticas Medioambientales y Tecnológicas, Spain), Enresa (Empresa Nacional de Residuos Radiactivos, Spain), Nagra (National Cooperative for the Disposal of Radioactive Waste, Switzerland), KAERI (Korea Atomic Energy Research Institute, Korea), ONDRAF/NIRAS (Organisme National des Déchets Radioactifs et des Matières Fissiles Enrichies, Belgium), Posiva (Posiva Oy, Finland), SKB (Swedish Nuclear Fuel and Waste Management Company, Sweden). The project was further supported by the E.U. Directorate General XII, Science, Research and Development, and the Swiss Federal Ministry of Science and Technology.

Many research groups have contributed to the FEBEX experiments. Major contributors that have been involved for the purpose of this report are UDC (Universidade de La Coruña, Spain), and UPC (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, Spain).



Location of Nagra's underground test facility at the Grimsel Pass in the Central Alps (Bernese Alps) of Switzerland

## Grimsel area (view to the west)

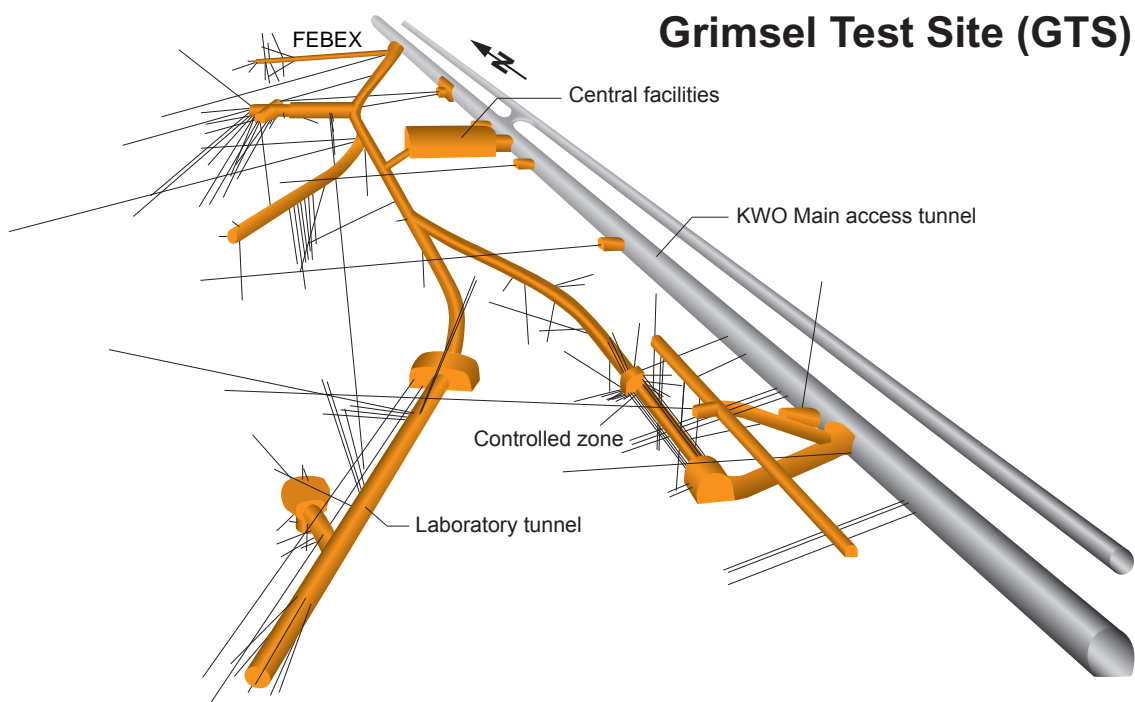


1 Grimsel Test Site








2 Lake Raeterichsboden

3 Lake Grimsel

4 Juchlistock

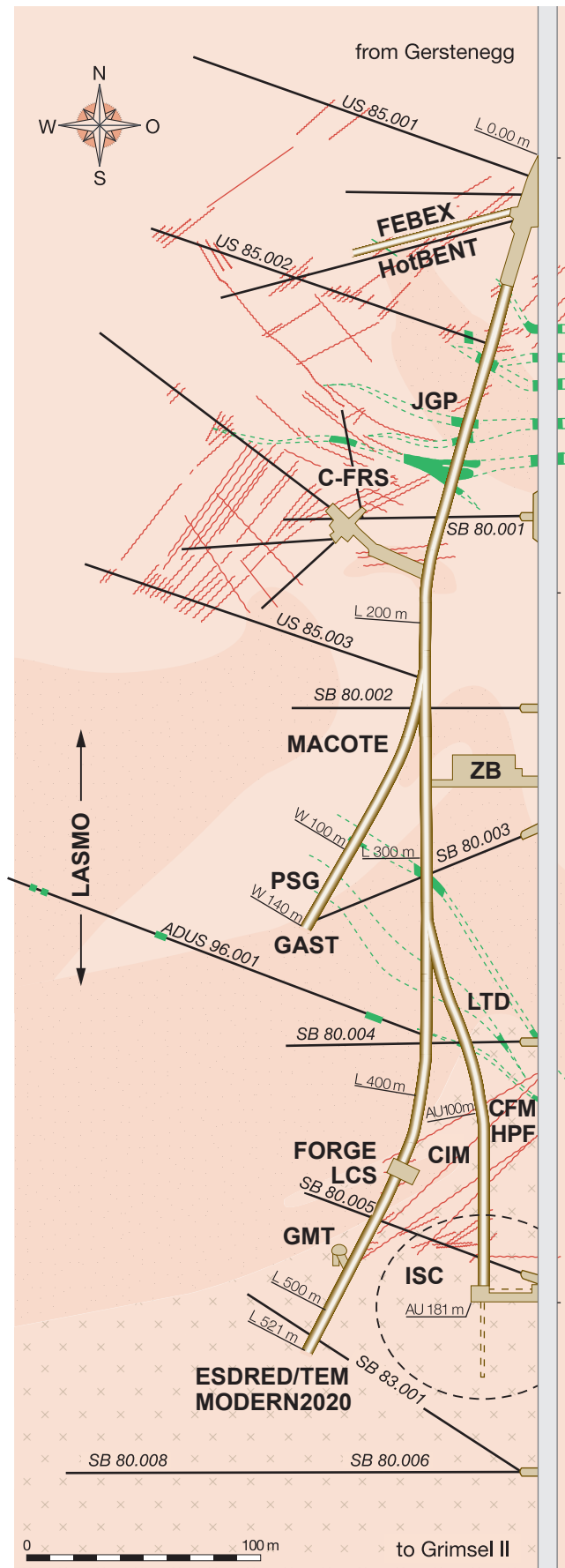


# Grimsel Test Site GTS

-  KWO-Access tunnel
-  Laboratory tunnel
-  Central Aaregranite (CAGR)  
High biotite content CAGR
-  Grimsel-Granodiorite
-  Shear zone
-  Lamprophyre
-  Main investigation borehole
- ZB** Central facilities

## GTS Phase VI 2003-2018

- CFM** Colloid Formation and Migration
- C-FRS** Criepti Fractured Rock Studies
- CIM** C-14 / I-129 Migration through aged cement
- ESDRED/TEM** Test and Evaluation of Monitoring Systems
- FEBEX** Full-scale Engineered Barriers Experiment
- FORGE** Fate of Repository Gases
- GAST** Gas-permeable Seal Test
- GMT** Gas Migration Test in the EBS
- HotBENT** High Temperature Bentonite project
- HPF** Hyperalkaline Plume
- ISC** In-situ Stimulation and Circulation Project
- JGP** JAEA Grouting Project
- LASMO** Large Scale Monitoring
- LCS** Long-Term Cement Studies
- LTD** Long Term Diffusion
- MACOTE** Material Corrosion Test
- MODERN2020** Development and Demonstration of Monitoring Strategies and Technologies
- PSG** Pore Space Geometry





## Abstract

The main objectives of the Full-Scale Engineered Barriers Experiment (FEBEX) were to demonstrate the practicality of implementing a horizontal disposal concept for high-level waste (HLW) in a crystalline host rock, validate the performance of the engineered barrier system (EBS), and enhance the understanding of coupled thermo-hydro-mechanical (THM) and geochemical (THMC) processes in the engineered and natural barriers.

The key element of the FEBEX project is the full-scale In Situ Test at the GTS, where two heaters simulating HLW canisters were emplaced within a buffer of pre-compacted bentonite blocks. From the start of heating in 1997, a constant temperature of 100 °C was maintained at the heater surface while the bentonite buffer slowly hydrated with water from the granite host rock. The evolution of temperature, water saturation, relative humidity, total pressure, pore pressure and displacement was monitored by a total of 632 sensors placed in the bentonite buffer and the geosphere. In 2002, after five years of heating, the EBS around Heater # 1 was dismantled and characterised while Heater # 2 remained in operation.

As an independent reference, a ~ 1:3 scale Mock-up Test has been run under controlled laboratory conditions at CIEMAT in Madrid. In contrast to the In Situ Test, water in the Mock-up is supplied at constant pressure to the buffer via a geotextile to assure well-defined experimental boundary conditions. The sensor density in the Mock-up is significantly higher than in the In Situ Test. These two large-scale FEBEX tests are complemented by extensive laboratory and modelling programmes.

Over the fifteen years since emplacement the EBS has largely performed as expected. The major processes and couplings affecting the buffer saturation during the initial thermal period had been identified prior to the start of the experiment. Much of the buffer, in both the In Situ and Mock-up Tests, achieved high saturation and significant swelling pressures developed throughout the greater part of the buffer. Buffer inhomogeneity due to construction played a smaller role than expected and a relatively uniform axisymmetric thermal, saturation and stress response controlled by distance from the heater has been observed. For the In Situ Test, this implies that the saturation process has been controlled by the low permeability of the saturated bentonite rather than heterogeneity of the more permeable rock mass.

THM modelling has played a significant role in the FEBEX programme from the initial design studies through the experimental period. The success of the models in predicting the initial development and continued evolution of the In Situ Test and the Mock-up relies on the identification of the most significant processes, detailed laboratory characterisation of the buffer, the limited influence of buffer heterogeneity (e.g. construction joints), and for the In Situ Test, the lack of sensitivity to geosphere heterogeneity. However, the limits of modelling (and of the datasets from the large-scale tests) have also been identified in terms of the ability to discriminate between additional processes which may influence the final part of the saturation process.

A significant improvement in THC/THMC modelling of the clay barrier has been achieved during the FEBEX project. Throughout the course of the project, THC/THMC codes were developed which could handle the observed thermo-hydro-geochemical couplings and account for the most relevant features of the THC conceptual model.

In summary, the FEBEX In Situ and Mock-up Tests have provided a unique insight into the EBS evolution at a realistic scale and over a time frame of 15 years, covering a significant part of the early EBS evolution in a repository. Demonstration of the practicality of the concept was achieved within the first few years with the construction and operation of the In Situ Test. The

development of a low permeability, highly saturated outer layer of the buffer with significant swelling pressures and the absence of any indication of preferential flow demonstrates the buffer's required performance over time as saturation increases. With the final dismantling of the In Situ Test in 2015, a wealth of information on the state of the buffer and on the action of corrosion, geochemical and microbial processes will be provided that extends the current process understanding of buffer evolution. The dataset will further constrain THM/THMC models and hence increase their long-term predictive capabilities.

## Zusammenfassung

Die Hauptziele des FEBEX-Experiments (Full Scale Engineered Barrier Experiment) waren der Nachweis der technischen Realisierung eines horizontalen Einlagerungskonzepts für hochaktive Abfälle (HAA) in einem kristallinen Wirtgestein, die Validierung der Eigenschaften von technischen Barrieren (EBS) sowie die Erweiterung des Verständnisses von gekoppelten thermo-hydromechanischen (THM) und thermo-hydrogeochemischen (THMC) Prozessen in den technischen und natürlichen Barrieren.

Den Kernpunkt des FEBEX-Projekts bildet ein In situ-Grossversuch im Felslabor Grimsel (FLG), in dem zwei Heizelemente, welche eingelagerte Behälter simulieren, innerhalb einer technischen Barriere von vorverdichteten Bentonitblöcken eingebaut wurden. Seit Beginn des Experiments im Jahr 1997 wurde an der Heizelementoberfläche eine konstante Temperatur von 100 °C erzielt, währenddessen sich die Bentonitverfüllung langsam mit Wasser aus dem umgebenden Granitgestein aufsättigte. Die Entwicklung der Temperatur, der Aufsättigung, der relativen Feuchtigkeit, des Gesamtdrucks, des Porendrucks und der Verschiebungen innerhalb der Bentonitbarriere und der Geosphäre wurde durch insgesamt 632 Sensoren überwacht. Nach fünf Jahren Laufzeit wurde das Heizelement 1 im Jahr 2002 abgeschaltet, ausgebaut und analysiert, während das Heizelement 2 in Betrieb blieb.

Zeitgleich wurde ein skaliertes Versuch (im Massstab 1:3, "Mock-up"-Versuch) in den Labors von CIEMAT in Madrid unter kontrollierten Laborbedingungen durchgeführt. Im Gegensatz zum In situ-Versuch wurde der Mock-up-Versuch bei konstantem Wasserdruck und definierten experimentellen Randbedingungen über ein Geotextil aufsättigt. Die Sensordichte im Mock-up-Versuch war deutlich höher als im In situ-Versuch. Diese beiden FEBEX-Versuche werden durch umfangreiche Labor- und Modellierprogramme ergänzt.

Seit dem Einbau vor 15 Jahren verhält sich die technische Barriere weitestgehend wie erwartet. Bereits vor Beginn des Experiments wurden die Hauptprozesse und -interaktionen in der technischen Barriere während der frühen Heizphase identifiziert. Der Grossteil der Bentonitbarriere, sowohl beim In situ- wie beim Mock-up-Versuch, erreichte einen hohen Sättigungsgrad und erhebliche Quelldrücke. Inhomogenitäten in der Bentonitbarriere, bedingt durch deren Einbau, spielten eine untergeordnete Rolle. Dadurch war zu beobachten, dass die Wärmeausbreitung, Aufsättigung und der Spannungsaufbau relativ gleichmässig und achsensymmetrisch verliefen und massgeblich durch den Abstand zu den Heizelementen gesteuert wurden. Für den In situ-Versuch bedeutet dies, dass der Aufsättigungsprozess durch die geringe Permeabilität des gesättigten Bentonits, statt durch Heterogenitäten im durchlässigeren Umgebungsgestein kontrolliert wurde.

Im FEBEX-Programm wurde der THM-Modellierung bereits von den ersten Designstudien bis über den gesamten Versuchszeitraum eine bedeutende Rolle beigemessen. Der Erfolg der Modelle bei der Vorhersage der anfänglichen Experimentphase und der stetigen Weiterentwicklung der Bentonitbarriere des In situ- und des Mock-up-Versuchs basiert auf der Identifizierung der wichtigsten beeinflussenden Prozesse. Für den Erfolg ausschlaggebend waren zudem die detaillierte Charakterisierung des Bentonits im Labor, der begrenzte Einfluss der Heterogenität der Bentonitbarriere (z.B. Fugen zwischen den Bentonitblöcken) sowie die geringe Sensitivität gegenüber Heterogenitäten in der Geosphäre. Jedoch sind die Grenzen der Modellierung (und der generellen Nutzung von Datensätzen aus Grossversuchen) aufgezeigt worden. Speziell zu erwähnen ist dabei eine Limitierung bei der Beschreibung von weiteren Prozessen, die im Endstadium des Aufsättigungsprozesses auftreten können.

Ungeachtet dessen ist eine signifikante Verbesserung der THC/THMC-Modellierung der Tonbarriere im Rahmen des Projekts FEBEX erreicht worden. Im Laufe des Projekts wurden THC/THMC-Codes entwickelt, welche die beobachteten thermo-hydro-geochemischen Interaktionen erfassen sowie die wichtigsten Merkmale des THC-Verhaltens in konzeptionellen Modellen widerspiegeln können.

Zusammenfassend wird festgehalten, dass die FEBEX In situ- und Mock-up-Versuche einen einzigartigen Einblick in die Entwicklung einer Bentonitbarriere im realistischen Massstab ermöglicht haben. Der Beobachtungszeitraum von 15 Jahren deckt dabei einen bedeutenden Teil der frühen Entwicklung einer technischen Barriere in einem geologischen Tiefenlager ab. Die Machbarkeit wurde bereits in den ersten Jahren mit dem Aufbau und der ersten Betriebsphase des In situ-Tests demonstriert. Die geforderten Eigenschaften der technischen Barriere konnten anhand des Erreichens einer geringen Durchlässigkeit, des hohen Aufsättigungsgrads der äusseren Barrierschicht sowie der signifikanten Quelldrücke aufgezeigt werden. Zudem wurden keine bevorzugten Fliesspfade nachgewiesen. Mit dem Ausbau des letzten Heizelements beim In situ-Versuch im Jahr 2015 werden wertvolle zusätzliche Informationen über den Zustand der Bentonitbarriere und die langfristigen Auswirkungen auf Korrosion, geochemische und mikrobielle Prozesse gewonnen. Diese werden das Prozessverständnis des Verhaltens von technischen Barrieren erweitern. Der Datensatz wird zudem die Weiterentwicklung der THM/THMC-Modelle ermöglichen und somit die Verlässlichkeit für längerfristige Vorhersagen erhöhen.

## Résumé

Le projet FEBEX (*Full-Scale Engineered Barriers Experiment*) avait pour objectifs principaux de démontrer la faisabilité du stockage horizontal des déchets de haute activité (DHA) dans une roche d'accueil cristalline, de valider la performance du système de barrières ouvragées (EBS, *engineered barrier system*) et d'améliorer la compréhension actuelle des processus thermo-hydro-mécaniques (THM) et géochimiques (THMC) dans les barrières ouvragées et naturelles.

Le projet FEBEX est articulé autour de l'essai *in situ* à l'échelle 1:1 réalisé au Laboratoire souterrain du Grimsel, dans lequel deux corps de chauffe simulant la présence de conteneurs DHA ont été mis en place et entourés de blocs de bentonite précompactée. Dès le début de la phase de chauffe, en 1997, une température constante de 100 °C a été maintenue à la surface des corps de chauffe pendant la lente hydratation de la bentonite par l'eau provenant de la roche granitique environnante. L'évolution respective de la température, de la saturation en eau, de l'humidité relative, de la pression totale, de la pression interstitielle et du déplacement a été contrôlée au moyen de 632 capteurs placés dans la bentonite et la géosphère. En 2002, après cinq ans de chauffe, l'EBS enveloppant le corps de chauffe n° 1 a été démantelé et étudié, le corps de chauffe n° 2 restant en fonctionnement.

À titre de référence indépendante, un mock-up à l'échelle d'environ 1:3 a été réalisé en conditions de laboratoire contrôlées au CIEMAT, à Madrid. Dans le mock-up, au contraire de l'essai *in situ*, la pression de l'eau parvenant dans la bentonite était maintenue constante par le biais d'un géotextile, pour assurer des conditions cadres bien définies. Le mock-up était doté d'un nombre considérablement plus élevé de capteurs que l'essai *in situ*. En complément de ces deux essais FEBEX à grande échelle, un vaste programme d'essais en laboratoire et d'essais de modélisation a été mis en place.

Au cours des quinze années de l'expérience, les performances de l'EBS ont largement répondu aux attentes. Les principaux processus et comportement couplés affectant la saturation de la bentonite au cours de la phase thermique initiale avaient été identifiés avant le début de l'expérimentation. Dans les deux essais, *in situ* et sur mock-up, et pour une grande part de la bentonite, un degré de saturation élevé a été atteint et une pression de gonflement significative a pu être constatée. Le manque d'homogénéité de la bentonite, en rapport avec la construction de l'expérience, a joué un rôle moins important que prévu, et les mesures de contrainte, saturation et température relevées en fonction de la distance du corps de chauffe se sont avérées relativement uniformes, présentant une certaine symétrie axiale. Pour l'essai *in situ*, ces résultats signifient que le processus de saturation a été dominé par la faible perméabilité de la bentonite saturée plutôt que par l'hétérogénéité de la masse rocheuse, plus perméable.

La modélisation des phénomènes THM a joué un rôle important dans le programme FEBEX, tant au cours des études de conception initiales que durant la période d'expérimentation. Les modèles ont été en mesure de prédire efficacement le développement initial et l'évolution continue de l'essai *in situ* et sur mock-up. Ceci a été rendu possible par l'identification des processus principaux, la caractérisation détaillée de la bentonite en laboratoire, la limitation de l'impact de l'hétérogénéité de la bentonite (présence de joints de construction, par exemple) et, pour l'essai *in situ*, l'absence d'impact de l'hétérogénéité de la géosphère. La modélisation (et les données des essais à grande échelle) ont cependant montré leurs limites lorsqu'il s'agit de différencier les processus susceptibles d'influencer la phase finale du processus de saturation.

La modélisation THC/THMC de la barrière d'argile a connu une amélioration significative au cours du projet FEBEX. Tout au long du projet, des codes THC/THMC ont été élaborés afin de traiter les couplages thermo-hydro-géochimiques observés, tout en incorporant les aspects importants du modèle conceptuel THC.

En résumé, les essais FEBEX *in situ* et sur mock-up ont permis d'obtenir pour la première fois un aperçu de l'évolution de l'EBS à échelle réelle et sur une période de 15 ans, ce qui correspond à une part importante des premières phases de l'évolution de l'EBS dans l'environnement du dépôt. La démonstration de la mise en oeuvre du concept a été réalisée au cours des premières années du projet, durant les phases de construction et d'opération de l'essai *in situ*. Le développement dans la bentonite d'une couche externe caractérisée par une faible perméabilité, un haut degré de saturation, des pressions de gonflement importantes et l'absence de toute indication d'écoulement préférentiel, démontre une performance de la bentonite conforme aux attentes au cours du temps, à mesure de l'augmentation du degré de saturation. Le démantèlement final de l'essai *in situ* en 2015 sera par ailleurs l'occasion d'acquérir de nombreuses informations sur l'état des blocs de bentonite, l'action de la corrosion, ainsi que les processus géochimiques et microbiens, et de mieux appréhender le processus d'évolution de la bentonite mise en place autour des conteneurs. Les données viendront en outre renforcer les modèles THM/THMC et ainsi améliorer leurs capacités prédictives au long terme.

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# 1 Introduction

This report gives an overview of the contribution of the Full-Scale Engineered Barriers Experiment (FEBEX) to the understanding of the near-field of a repository for high-level radioactive waste. The aim is to provide a broad overview of activities and results rather than to analyse specific aspects of the different tests.

## 1.1 The FEBEX experiment

The FEBEX experiment was based on the Spanish reference concept for disposal of radioactive waste in crystalline rock (AGP Granito<sup>1</sup>, see Fig. 1-1), where waste canisters are placed horizontally in drifts and surrounded by a clay barrier constructed from highly compacted bentonite blocks (Enresa 1995, 2000). Other horizontal emplacement concepts for disposal of high-level waste (HLW) in crystalline rocks have been proposed in Project Gewähr (Nagra 1985), H12 (JNC 2000) and KBS-3H (Autio et al. 2007). A vertical emplacement concept KBS-3V (SKB 2011) is the current reference disposal concept in Sweden, Finland and South Korea. In clay rocks, horizontal emplacement concepts have been developed by both Nagra (2002) and Andra (2005).

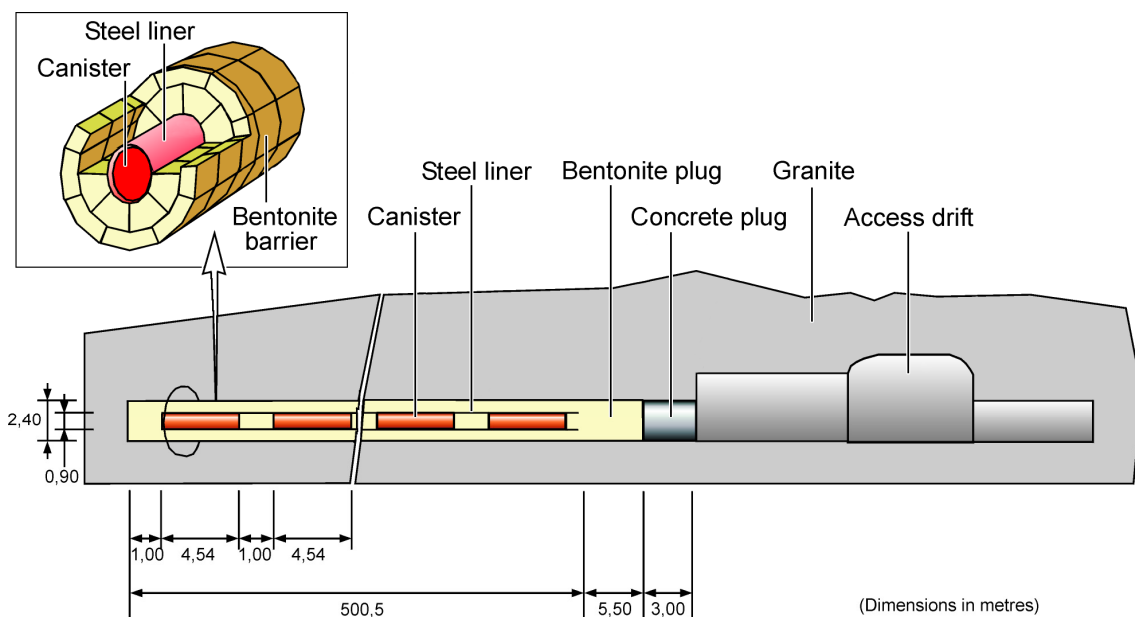


Fig. 1-1: Schematic of Spanish disposal concept for High Level Waste: AGP Granito.

FEBEX was the first full-scale demonstration experiment of a HLW disposal system. A full-scale test of spent fuel storage in vertical deposition holes had been previously performed at the Climax site, Patrick (1986), while the Buffer Mass Test, Pusch et al. (1985), was a 1 : 2 scale deposition hole experiment. Full-scale experiments have since been performed for AECL's HLW Concept (Buffer Container Experiment, Dixon et al. 2002) and the KBS-3V concept in the Prototype Repository Experiment at the Äspö Hard Rock Laboratory (SKB 2012). Demonstration of Nagra's concept for the Opalinus Clay has been investigated at 1 : 2 scale (Gaus et al. 2014) and a full-scale test is currently under way in the Full Scale Emplacement Experiment (FE) at the Mont Terri rock laboratory (Müller et al. 2012).

<sup>1</sup> Almacenamiento Geológico Profundo en Granito.

FEBEX comprises the full-scale In Situ Test at the Grimsel Test Site (GTS), a large-scale Mock-up Test, a supporting laboratory test programme and modelling activities. The Mock-up is performed in laboratory conditions at CIEMAT in Madrid (Martín & Barcala 2005). A similar experiment had previously been performed from 1990 to 1992 at Tokai Works, Japan Nuclear Cycle Development Institute (Big Bentonite Experiment, Chijimatsu et al. 2000). The OPHELIE Mock-up (Verstricht & Dereeper 2003) was carried out between 1997 and 2002 at the EURIDICE URL in Belgium. Similar tests have since been developed in the Czech Republic from 2002 (Mock-up-CZ, Pacovský et al. 2007), Korea from 2005 (KENTEX, Lee et al. 2006) and more recently in China (China Mock-up, Wang 2010, Chen et al. 2012). The FEBEX Mock-up is, however, the longest running and most highly instrumented test.

## 1.2 Project history and institutional framework

Over the period from initial design to the current day FEBEX has operated under five different institutional frameworks as listed in Tab. 1-1. The project was led by Enresa during FEBEX I, II and NF-PRO. FEBEX I and II were supported by Enresa and the E.U. Directorate General XII, Science, Research and Development and the Swiss Federal Ministry of Science and Technology (BBW). The FEBEX I partners were Enresa, BGR, Nagra and SKB. Additional partners for FEBEX II included Posiva, Andra, and ONDRAF/NIRAS. From 2008 to 2014, FEBEX has been part of the FEBEXe Project (partners are CIEMAT, KAERI, Nagra, Posiva and SKB) within the GTS Phase VI Programme. The final dismantling of the In Situ Test was performed as part of the FEBEX-DP project.

Tab. 1-1: Project history of FEBEX.

Project	Time	Activities
FEBEX I	1995 – 1999	Design, construction with heating initiated in 1997
FEBEX II	2000 – 2004	Continued saturation and partial dismantling of In Situ Test (2002)
NF-PRO	2005 – 2007	Continued saturation
FEBEXe	2008 – 2014	Ongoing saturation and planned final dismantling for In Situ Test
FEBEX-DP	2014 – 2017	Final dismantling of the In Situ Test

The major milestones for the In Situ Test were:

- 25/10/95: Start of tunnel boring machine excavation of FEBEX tunnel
- 01/07/96: Start of FEBEX Engineered Barrier System (EBS) construction
- 15/10/96: End of EBS construction
- 27/02/97: Start of heating<sup>2</sup>
- 28/02/02: Switch-off of Heater # 1
- 02/04/02: Start of partial dismantling
- 26/07/02: End of partial dismantling
- 24/04/15: Switch-off of Heater # 2
- 05/08/15: Completion of dismantling

<sup>2</sup> It was decided to allow the system to equilibrate after installation of the plug prior to the start of heating.

Since July 2002 the heating and ongoing saturation have been maintained apart from some short power interruptions with a maximum length of 7 days (06/02/03 – 13/02/03). Heater # 2 was switched off on 24/04/15 (6'630 days after the start of heating). The In Situ Test has now been fully dismantled and laboratory analyses of samples are ongoing.

The Mock-up Test has been in continuous operation since 04/02/97. The only disturbance to ongoing saturation was an overheating event that occurred in November 2000 and lasted for approximately 36 hours when heater temperatures peaked at over 200 °C. The chronology of the two large-scale tests is illustrated in Fig. 1-2.

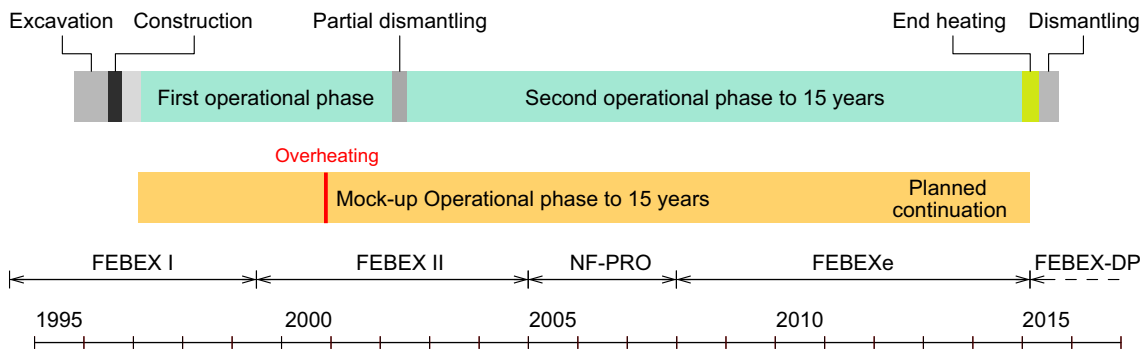


Fig. 1-2: FEBEX project timeline showing In Situ (green) and Mock-up operation (orange) and the different institutional frameworks.

## 1.3 Aims and objectives

### 1.3.1 Objectives of FEBEX I and II

The aims of the FEBEX I project (Enresa 2000) were:

- to demonstrate the feasibility of manufacturing, handling and constructing the engineered barriers
- to develop codes for the thermo-hydro-mechanical and thermo-hydro-geochemical performance assessment of a deep geological repository for high level radioactive wastes

The following three objectives were established:

1. Demonstration of the feasibility of handling and constructing an engineered barrier system.
2. Study of the thermo-hydro-mechanical (THM) processes in the near-field.
3. Study of the thermo-hydro-geochemical (THG) processes in the near-field.

The feasibility was demonstrated by the construction<sup>3</sup> and operation of the In Situ Test and further supported by the results from partial dismantling in 2002.

While it was concluded that "relevant progress in knowledge of the behaviour of the near-field could be achieved only by means of a very complete experiment, such as FEBEX", it was also

<sup>3</sup> The demonstration is partial as the bentonite block sizes and installation methods differ from those in the reference concept.

felt that the development, verification, and validation of the numerical models required a less complex system than the In Situ Test and this was in part the motivation for the Mock-up Test, and supporting laboratory tests (Enresa 2000). The demonstration objective of FEBEX was expected to be primarily attained by the In Situ Test and the main objectives of the Mock-up were to:

- gain knowledge and understanding of the long-term behaviour of a clay barrier under well controlled thermal and hydraulic gradients
- validate and verify the near-field THM models under controlled boundary conditions

The key differences between the Mock-up and In Situ Tests relate to the control and measurement of hydration and the outer thermal boundary conditions provided by the Mock-up together with its higher density of instrumentation. Differences in test geometry are discussed in Section 1.4.4.

FEBEX I and II were reported in a series of reports listed in Appendix A.

At the end of FEBEX II the behaviour of the instrumentation and heating systems of both tests had shown a high reliability, confirmed by results from partial dismantling of the In Situ Test, and it was felt advisable to continue with the large-scale tests for as long as possible (Enresa 2006a). It was also felt that an extension in time would benefit THM modelling by allowing a comparison with a longer dataset where data trends would be clearer and more consistent (variability between sensors was expected to decrease with time).

### 1.3.2 Objectives of NF-PRO

NF-PRO focussed on the "investigation of the detailed processes taking place in the near-field as well as their couplings in view of integration in performance assessment" (European Commission 2008). Amongst the detailed objectives of NF-PRO were:

- to establish a comprehensive insight in the chemical processes and materials interactions taking place in the near-field of a geological repository for HLW and spent-fuel disposal
- to investigate the evolution of the thermal, the hydrological and the mechanical processes taking place in the near-field and their influence on the total system
- to identify and to provide key data on critical processes and their couplings determining the evolution of the near-field and affecting radionuclide release to the geosphere
- to translate models and data on complex and coupled near-field processes to concise but accurate models and data as input to assessments of the overall system performance

NF-PRO supported the ongoing In Situ, Mock-up and laboratory experiments (Villar & Gómez-Espina 2007, Villar et al. 2008, Fernández & Villar 2010) and modelling studies including the extension of classical THM formulations (Sánchez et al. 2007). In addition, Time Domain Reflectometry (TDR) monitoring of saturation for the In Situ Test was refined and optimised. The work of NF-PRO is reported in a summary report and as a series of deliverable reports as listed in Appendix A.

Participation within NF-PRO extended the saturation period of the two experiments by three years, building confidence in previous observations. Information was, however, still limited because of the slow natural evolution of the system.

### 1.3.3 Objectives of FEBEXe

The objectives of FEBEXe were to develop a more detailed understanding of early-time coupled processes needed to predict near-field evolution. Particular aspects included:

- the evolution of thermal conductivity of the partially saturated buffer
- the role of thermal convection
- the onset of corrosion and consequent gas production
- gas transport capacity of the near-field (saturation history)
- the geochemical evolution of the near-field (e.g. iron/bentonite interactions)

This was motivated by the longer than expected time required for buffer saturation together with the identification of additional uncertainties regarding coupled processes within the buffer.

Originally it had been planned to extend saturation to 2012 but this was subsequently further extended to continue heating until 2014 with final excavation in 2015 (see Fig. 1-2).

## 1.4 In Situ and Mock-up Test layout and instrumentation

### 1.4.1 FEBEX bentonite

The compacted buffer in both the In Situ and Mock-up Tests is constructed of FEBEX bentonite (also known as "Serrata" clay) extracted from the Cortijo de Archidona deposit, exploited by Minas de Gádor, S. A., in Serrata de Níjar (Almería, Spain). The deposit had been selected by Enresa prior to the FEBEX experiment as the most suitable material for the backfilling and sealing of a HLW repository. The reasons for selection were: very high montmorillonite content, large swelling pressure, low permeability, acceptable thermal conductivity, good retention properties and ease of compaction for the fabrication of blocks (Enresa 2000).

Tab. 1-2: Bentonite main mineral content as percentages for FEBEX, S-2 (Enresa 2000) and MX-80 R1 (SKB 2011) bentonites.

Mineral (%)	FEBEX bentonite	Bentonite S-2	MX-80 R1
Smectite	92 ± 3	92 ± 4	84 ± 3
Quartz	2 ± 1	2 ± 1	3 ± 1
Plagioclase (Na, Ca)	3 ± 1	3 ± 1	--
Cristobalite	2 ± 1	2 ± 1	0 – 1
Feldspars	Traces	--	4 ± 2
Calcite	1 ± 0.5	1 ± 1	0 – 1

The deposits at Serrata de Níjar were formed after volcanism associated with Neogene geotectonics, which occurred between 15 and 18 Ma. Subsequent episodes of emersion and immersion, together with ongoing volcanic activity contributed to the alteration of the volcanic rocks into silica, alunite, jarosite, kaolinite or bentonite according to the composition of the solutes. The mineralogy of the FEBEX bentonite, Bentonite S-2 (a related bentonite from the same deposit) and MX-80 R1 (the reference bentonite for SKB's SR-SITE) are given in Tab. 1-2.

Extensive characterisation of the FEBEX bentonite with special emphasis on the influence of temperature is documented in Enresa (2000, 2006b, 2006c), Lloret et al. (2003), Villar & Lloret (2004), Fernández et al. (2004), Fernández & Rivas (2005), Lloret & Villar (2007) and Villar et al. (2010).

Laboratory characterisation of FEBEX bentonite for selection and preparation included:

- mineralogical composition (including XRD and SEM<sup>4</sup>)
- chemical composition
- identification properties: liquid & plastic limit, plasticity index, grain size distribution, specific surface and equilibrium water content
- pore size distribution and fabric
- cation exchange capacity
- surface charge density
- redox capacity

#### **1.4.2 Location and geological setting of the In Situ Test**

The In Situ Test is located within the FEBEX drift at the Grimsel Test Site (GTS). The GTS is located at an elevation of about 1'730 m a.s.l., roughly 400 to 450 m beneath the Juchlistock mountain top in Central Switzerland. The host rocks are the leucocratic Central Aare Granite and Grimsel Granodiorite in the southern section of the Central Aar Massif. During the Alpine Orogeny (40 Ma), Aare Granite was subject to regional shear displacement and weak to intermediate metamorphism. The latter caused significant foliation whereas the shear movement resulted in the development of cataclastic and mylonitic shear zones. Within the GTS area up to twelve different shear and fracture sets can be observed in detailed drill core and surface evaluations (Keusen et al. 1989). The most important geological features in this environment are the two families of shear zones (K and S). Two large S-family shear zones have been assumed to act as the hydraulic boundaries of the FEBEX site. The inflows to the tunnels from these shear zones were approximately 60 and 23 mL/min respectively before installation (Alonso & Alcoverro 2005).

Extensive hydraulic testing in existing and new boreholes was performed as part of the FEBEX project. Tests included pressure build-up, pulse tests and longer production/injection tests. The tests are documented in Meier et al. (1995) and Guimerà et al. (1996, 1998). Larger scale hydraulic tests were performed in boreholes BOUS 85.001, BOUS 85.002, FBX 95.001, and FBX 95.002 (see Fig. 1-3a). The extensive hydraulic testing together with monitoring of the response to excavation was used to identify the most important hydraulic structures and their connectivity.

The major hydraulic feature that intersects the FEBEX drift is associated with the lamprophyre dyke that intersects close to Heater # 1. Martínez-Landa & Carrera (2005, 2006) suggest that hydraulic conductivity of the background rock (matrix and small fractures) is  $\sim 10^{-11}$  m/s, while locally, features such as Fr-7 (lamprophyre channel see Fig. 1-3b and Map 1) are many orders of magnitude more permeable. It should be noted however that the matrix permeability at GTS is believed to be typically higher than that of the saturated bentonite and higher than that expected for the crystalline matrix in repository sites such as Olkiluoto (Finland) and Forsmark (Sweden).

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<sup>4</sup> X-ray diffraction methods and scanning electron microscope.

Inflows to the drift were measured during and after excavation using a variety of methods. The total was estimated at 7.8 mL/min (Alonso et al. 2005, Martinez-Landa & Carrera 2005), approximately half of which came from 6 identified inflow points. The total drift inflow is significantly below the suggested maximum permitted inflow to a KBS-3V deposition hole of 100 mL/min (SKB 2011).

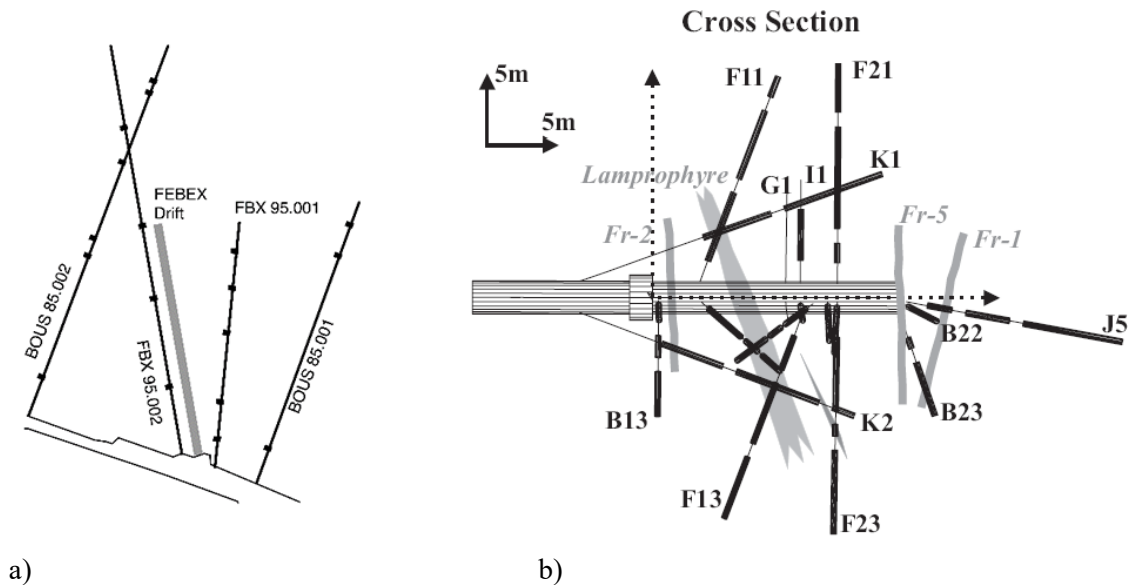


Fig. 1-3: Borehole geometry and packer locations: a) prior to gallery excavation (Meier et al. 1995) and b) during FEBEX experiment (Martinez-Landa & Carrera 2006).

Feature FR-7 is within the structure labelled Lamprophyre.

The experimental layout for the In Situ Test from 1996 – 2002 is shown in Fig. 1-4a. The FEBEX drift has a diameter of  $2.28 \pm 0.01$  m and a total length of 71.4 m. The original FEBEX test section extended from 54 to 71.4 m. The test section was isolated by a 2.7 m long, keyed-type cast concrete plug. Within the test section two 4.54 m long carbon steel heaters simulating the HLW canisters were emplaced within a steel liner and a buffer built of pre-compacted FEBEX bentonite blocks. The blocks were compacted to a dry density of  $\sim 1.7$  Mg/m<sup>3</sup> such that the achieved average dry density after emplacement was 1.6 Mg/m<sup>3</sup>. A cross-section of the block layouts is also shown in Fig. 1-4c. In 2002 Heater # 1 was excavated. The layout after excavation is shown in Fig. 1-4b.

The EBS was constructed as 136 vertical slices. The slices were numbered sequentially. Slices 1 – 3 were at the rear of the tunnel (17.39 – 17.3 m along the test section) and were adjusted to match the concave end of the tunnel. Slices 4 – 136 (next to plug) followed the patterns shown in Fig. 1-4c. Details of the slices can be found in Enresa (1998b). In all, the EBS was made up of a total of 5531 blocks. Each block weighed between 20 and 25 kg and five different block-shapes (named BB-G-01 to 05) were used to form the different slices (see Fig. 1-4c).

The central steel liner has a length of 10 m and extends over the EBS section containing the two heaters and the 1 m gap between them. The liner is of 15 mm-thick perforated steel with an inner diameter of 940 mm and provides the space into which the heaters are inserted (as required by the AGP Granito concept).

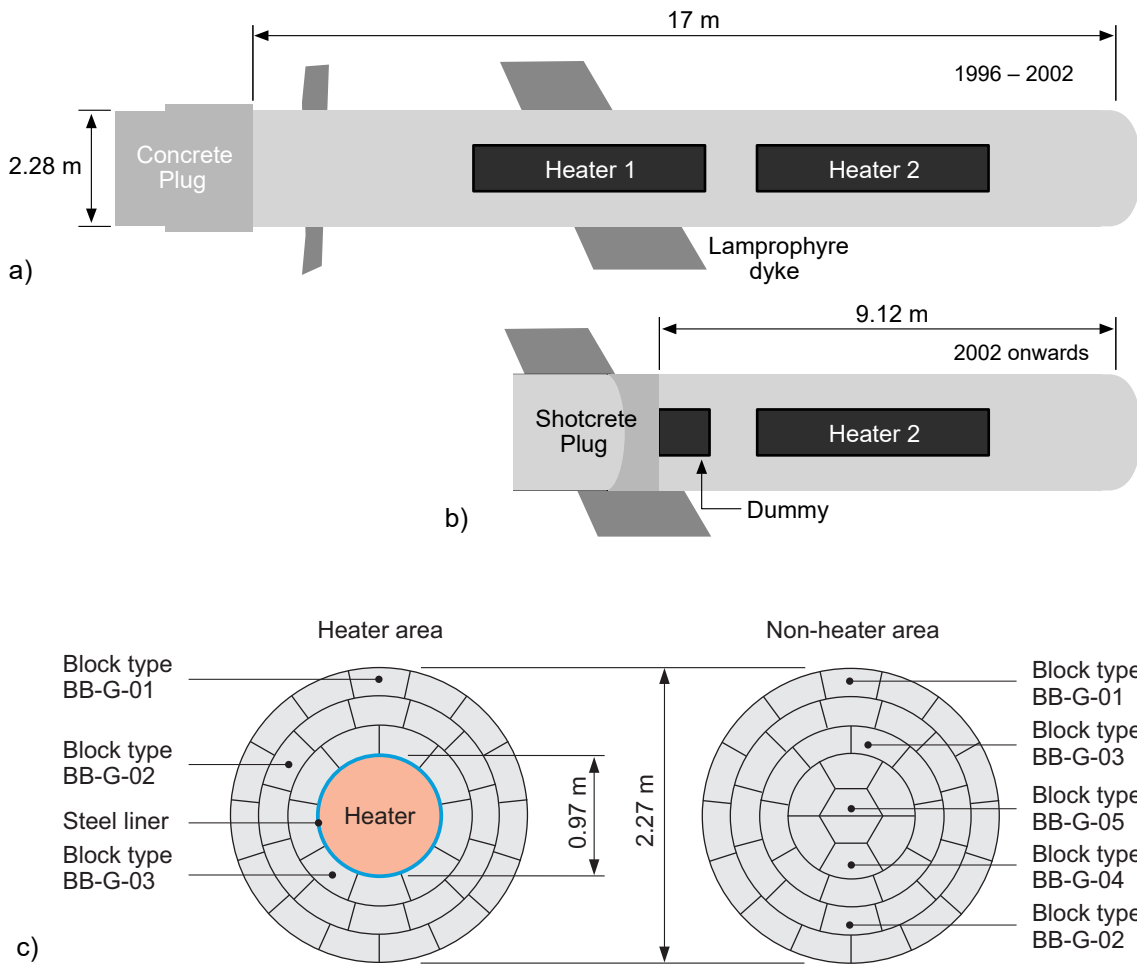


Fig. 1-4: a) FEBEX layout 1997 – 2002 prior to removal of Heater # 1, b) layout 2002 – 2015 and c) bentonite block vertical cross-sections.

Sensors in the buffer were arranged in a series of vertical cross-sections named A, B1, B2, C, D1, D2, E1, E2, F1, F2, G, H, I, K, L, M1, M2 and N. Sections with the same identifying letter (e.g. B1, B2) had identical sensor configurations. Geosphere sensors were located in BOUS 85.001, BOUS 85.002, FBX 95.001, and FBX 95.002 and 19 boreholes drilled from the drift. Other sensors, such as psychrometers and TDR probes were installed in shorter boreholes, drilled from the drift (up to 2.5 m).

Sensors were identified using a naming convention as AA-BBn-CC, where AA was the sensor type, BBn the location type and number (section number or borehole name) and CC. The order number of sensors within the section or borehole.

Six ceramic filter pipes were installed by GRS (Gesellschaft für Reaktorsicherheit) in the bentonite buffer around Heater # 1. The pipes were made of sintered ceramic with Teflon couplings in a protective perforated metal cover. After removal of Heater # 1, additional sensors were added along three new plastic pipes inserted into the buffer and at the interface with the plug (see Fig. 1-5b). New instrument sections were defined as O, P, Q, R, S, T and U. The P section corresponded to the new total pressure cells at the concrete/bentonite interface and S to temperature sensors (see Fig. 1-5b).

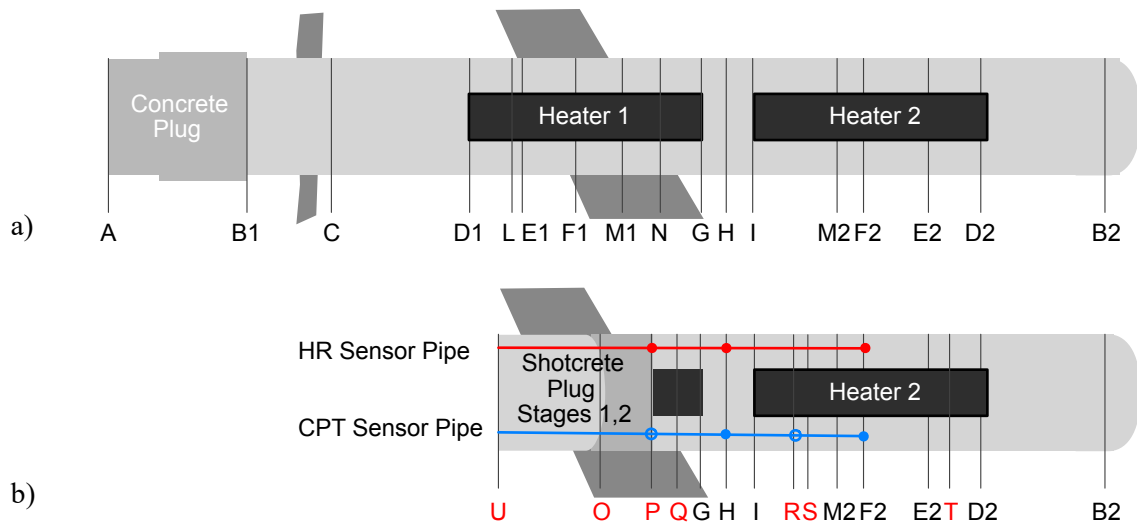


Fig. 1-5: a) FEBEX layout 1997 – 2002 showing instrumentation sections, b) layout 2002 – 2015 showing additional instrumentation sections (in red) and HR (relative humidity) and CPT (total pressure and thermocouple) pipes.

Three sintered stainless steel draining pipes were installed around Heater # 2. Each pipe contained 4 stainless steel tubes for gas extraction/injection. In addition, six pipes were installed in April 2003 to collect porewater from the bentonite. The pipes contained sintered porous 316L stainless steel at depths corresponding to Sections G, I and F2. Humidity sensors and filters to collect porewater from the bentonite were placed within each section giving 18 sampling points.

Specimens of steel, titanium and copper were located in the bentonite close to the heaters to study corrosion. Chemical tracers were also installed within the bentonite and at the boundaries. Tracers included: iodine, rhenium, selenium, boron, deuterium, europium, cesium, thorium, uranium, and neodymium. Five glass ampoules containing deuterium were included in blocks in the external ring of blocks close to the centre of Heater # 1 (instrumentation Section M1, dismantling Section S29), while other tracers were emplaced using the following methods: within sintered metallic capsules (labeled SSS), mixed with bentonite in plugs of compacted bentonite (CP), and in impregnated filter paper (FP).

In 2005, two boreholes (FUN 05.001, FUN 05.002) were drilled parallel to the FEBEX drift at distances of 30 and 60 cm, to investigate geochemical gradients and bentonite colloid concentrations in the near-field (Buil et al. 2010). Fracture transmissivity was typically very low:  $10^{-12} - 10^{-11} \text{ m}^2/\text{s}$  with the exception of interval FU1-1 intersecting a fracture with a transmissivity of  $6 - 8 \times 10^{-10} \text{ m}^2/\text{s}$  near to the end of the drift (known as the "September" fracture). This feature may be related to the fracture zone containing Fr-5 which was intersected by boreholes J5 and B23 (see Fig. 1-3b). Inflow from this feature may have caused some problems during installation (Guimera et al. 1998) although Svemar & Huertas (2004) suggest that there were no problems with inflow during construction of the FEBEX EBS.<sup>5</sup>

<sup>5</sup> In one very short section of the drift some plastic sheet was emplaced to protect the bentonite from water from a borehole mouth.

Tab. 1-3: Sensors installed at the time of construction of the FEBEX In Situ Test.

Measurement	Type	Count
Temperature	Thermo-couple	189
Total pressure	Vibrating wire	40
Water content	Capacitive, psychrometer, TDR	59, 76, 24
Hydraulic pressure	Borehole interval, packers, bentonite	62, 62, 52
Displacements	Vibrating wire, LVDT*, potentiometer	44
Heater	Resistor current and voltage	12
Gas pressure & flow	Gas & atmospheric measurements	12
Total at construction		632

\* Linear Variable Differential Transformer.

### 1.4.3 Mock-up Test

The FEBEX Mock-up Test is a near full-scale laboratory experiment performed at CIEMAT in Madrid (Martín & Barcala 2005, Martín et al. 2006). The layout is illustrated in Fig. 1-6. The heater and buffer layout is similar to the In Situ Test at a slightly reduced scale and without a central liner. The heaters are arranged symmetrically within a steel confining structure. Water is provided through inlets in the confining structure into a geotextile layer acting as a permeable interface to assure homogeneous water distribution. The Mock-up Test is highly instrumented with a higher density of temperature and total pressure cells than the In Situ Test (see Tab. 1-4).

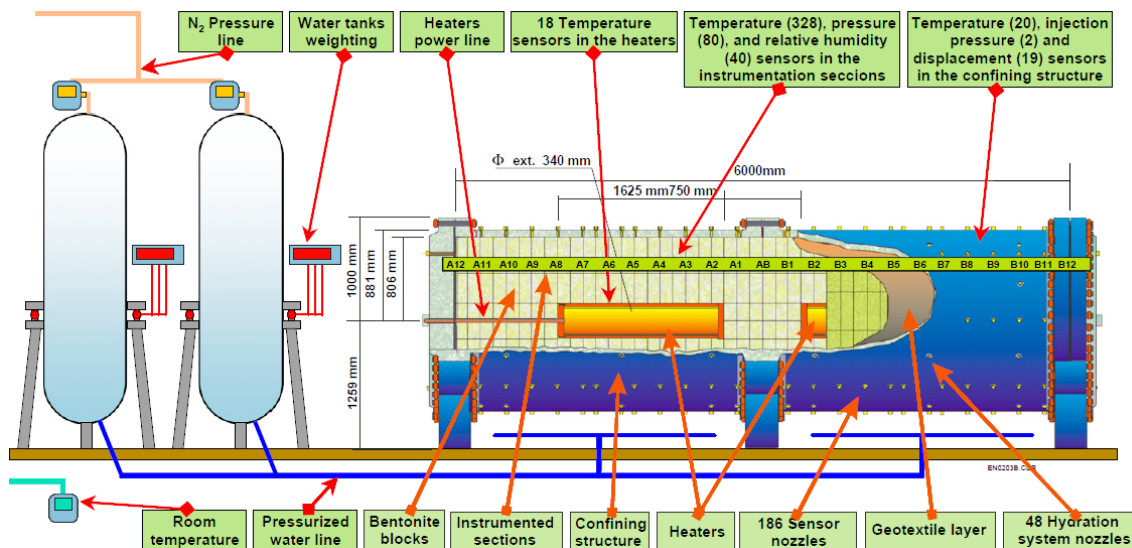


Fig. 1-6: Layout of Mock-up Test at CIEMAT (Madrid) (from Cañamón et al. 2004).

Tab. 1-4: Sensors in the FEBEX Mock-up Test (Martín et al. 2006, Martín &amp; Barcala 2011).

Measurement	Type of sensor/value	B	S	E	H	Total	Working (after 15 yrs)
Temperature	Thermoresistance	328	20	1	18	367	328
Total pressure: radial/tangential/axial	Semi-conductor strain	14/14/22				50	9/9/15
Relative humidity	Capacitive	40				40	20
Hydraulic pressure	Semi-conductor strain	20				20	13
Strains	Extensometric gauges		19			19	19
Water injection pressure	Silicon diaphragm		2	1		3	3
Heating power	Calculated			2		2	2
Total		438	41	4	18	501	418

B: Bentonite, S: Structure, E: External, H: Heater

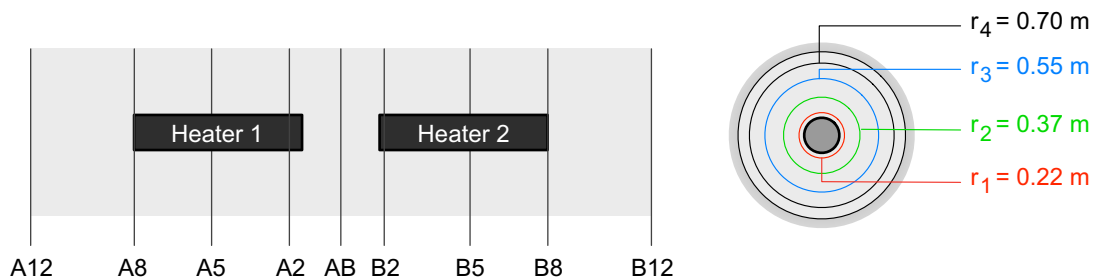


Fig. 1-7: Layout of Mock-up sensors showing selected vertical slices and radii 1 – 4 (colour coding as used in Mock-up Figures).

Instruments in the Mock-up are arranged on vertical slices located every 2 blocks and named A12, A11, ... B11, B12 with Slice AB located at the midpoint. Within each slice instruments are located at specific radii (0 – 4) as shown in Fig. 1-7. The sensor layout is symmetric about the central AB plane (i.e. the sensor layout at Slice Ax is identical to that at Slice Bx).

#### 1.4.4 Comparison of In Situ and Mock-up Tests

A major difference between the two tests is that in the Mock-up water is supplied at constant pressure to the buffer via the geotextile, while in the In Situ Test water is supplied by the geosphere. Effects of either limited or heterogeneous water supply could therefore only be seen in the In Situ Test (Martín et al. 2006)<sup>6</sup>. The pre-heating flooding of the Mock-up to fill joints/gaps is another potentially important difference between hydration of the two tests (see dis-

<sup>6</sup> Although the water supply from the granite was likely to be heterogeneous, it appears to have had no significant effect on the buffer hydration. The most probable reason is that hydration was controlled by the permeability of the bentonite, and the rock matrix supplied all the water required for buffer hydration (see discussion in Chapter 4).

cussion in Zheng & Samper 2008). Other differences relate to the absence of a central steel liner, the overall geometry (see Tab. 1-5) and buffer properties (see Tab. 1-6).

The In Situ Test was originally approximately 3 times longer and 40 % wider than the Mock-up (Fig. 1.9) resulting in a volume approximately 5.7 times larger. The mass of bentonite is only some 5.1 times greater due to the slightly lower bentonite dry density in the In Situ Test. With regard to the buffer, although there are minor differences in the initial conditions (water content and dry density) and block sizes, the overall buffer dry density is only slightly higher in the Mock-up (1.65 vs. 1.60 Mg/m<sup>3</sup>). This small difference does however influence the expected swelling pressure and hydraulic conductivity. Fig. 1-9 shows empirical regressions for these two properties from Enresa (2000). It can be seen that the swelling pressure is likely to be 30 % higher in the Mock-up Test based on the average dry density. Hydraulic conductivity is expected to be about 30 % lower. The difference between the properties of the as-compacted blocks is larger. Uncertainty on the regressions is estimated at ± 25 % for swelling pressure and ± 30 % for hydraulic conductivity.

Tab. 1-5: Geometry of In Situ and Mock-up Tests.

		<b>In Situ Test</b>	<b>Mock-up</b>	<b>Ratio</b>
Buffer length	(m)	17.4 (9.12 from 2002)	6	2.90
Buffer diameter	(m)	2.28	1.62	1.41
Heater length	(m)	4.54	1.63	2.79
Heater diameter	(m)	0.9 heater/0.97 liner	0.34	2.85
Buffer thickness	(m)	0.66	0.64	1.02
Gap between heaters	(m)	1	0.75	1.33
Total volume	(m <sup>3</sup> )	71.04	12.37	5.74
Buffer volume	(m <sup>3</sup> )	64.3	12.1	5.33
Buffer mass	(t)	115.7	22.5	5.14

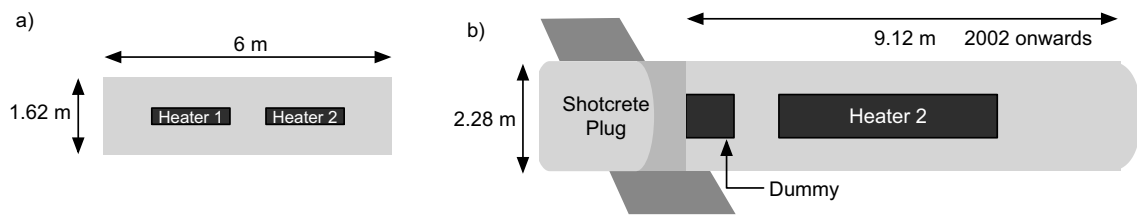


Fig. 1-8: Comparison of a) Mock-up and b) In Situ Test (after 2002) geometry.

Tab. 1-6: Bentonite block properties for In Situ and Mock-up Tests.

Property		In Situ Test	Mock-up
Water content of blocks prior to construction		14.4 %	13.8 %
Block dry density	(Mg/m <sup>3</sup> )	1.7	1.77/1.82 (core)
Average dry density	(Mg/m <sup>3</sup> )	1.60	1.65
Expected swelling pressure	(MPa)*	5.8	8.2
Percentage volume as construction gaps		5.5 %	6.5 %
Block weight (kg)		20 – 25	25/12.4 (core)
Number of blocks		5331	908
Number of slices		136	48

\* Calculated from empirical correlations (Enresa 2000) and average dry density.

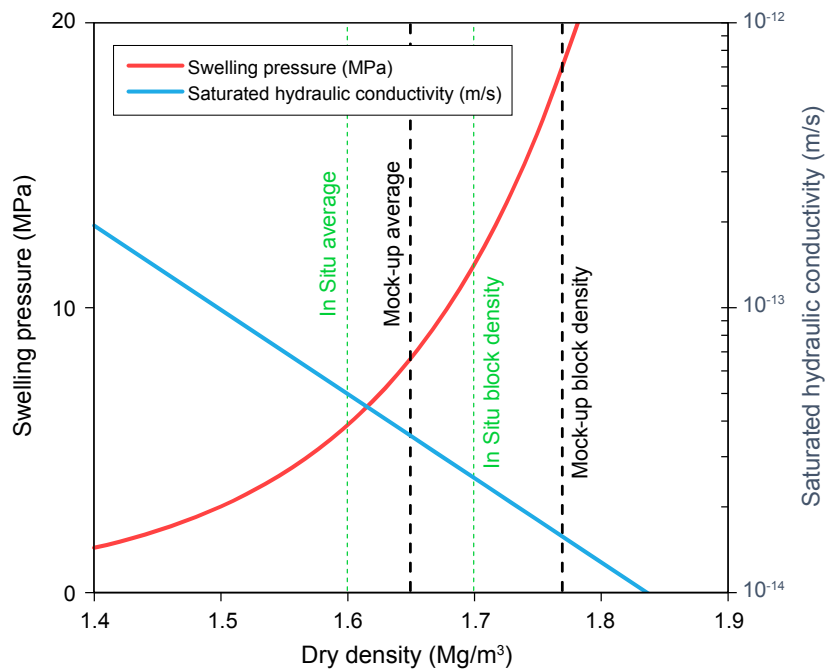


Fig. 1-9: Empirical regressions (from Enresa 2000) for swelling pressure and hydraulic conductivity with bentonite dry density.

Dashed vertical lines show the compacted block and average dry density for the two tests.

## 1.5 Modelling

Conceptual and numerical modelling of the FEBEX In Situ and Mock-up Tests has been a key part of the various projects since inception as demonstrated by the objectives set (see Section 1.3).

### 1.5.1 THM modelling

Thermo-hydro-mechanical (THM) modelling of the FEBEX In Situ Test can be considered under the following headings:

- Modelling during test design (Enresa 1996)
- Pre-operational modelling carried out before the start of the test (Enresa 1998a)
- Concurrent modelling to aid interpretation during the performance of the test (Enresa 2006a, 2006c, Gens et al. 2009)
- Modelling within the DECOVALEX III<sup>7</sup> programme (Alonso et al. 2005, Tsang et al. 2005)
- Additional modelling within FEBEXe (Dupray et al. 2013, Olivella et al. 2012)

Some "post-mortem" modelling has been performed after dismantling of the first part of FEBEX (Sánchez et al. 2012b, Olivella et al. 2012, Dupray 2013) but it is envisaged that further modelling will be performed after the final dismantling of the experiment. Modelling of the Mock-up has followed a largely similar path.

THM modelling in the FEBEX I & II projects was largely performed using the CODE\_BRIGHT numerical simulator (Olivella et al. 1996) by Universitat Politècnica de Catalunya (UPC). For the THM modelling of both tests an Operational Base Case (OBC) analysis was established. The OBC model attempts to incorporate all available information obtained from laboratory tests of FEBEX bentonite at the beginning of the operational stage. The use of the OBC has provided a reference case against which the performance of the two tests and alternative models can be considered.

During DECOVALEX a wider range of THM codes were used as part of a collaborative modelling exercise. During FEBEXe additional modelling has also been performed by EPFL using the LAGAMINE code (Dupray et al. 2013).

### 1.5.2 THC/THmC<sup>8</sup> modelling

Thermo-hydro-geochemical (THC/THmC) modelling was also performed within FEBEX I and II. The emphasis was on developing THC/THmC models of the main geochemical processes controlling the geochemical evolution of the clay barrier in terms of major ion composition, pH and alkalinity. Redox and interactions with corrosion products were not considered. Multiple conceptual models for the bentonite porewater (Samper et al. 2005a) have been developed based upon the two porewater datasets (from squeezing or aqueous extraction).

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<sup>7</sup> DECOVALEX, DEmonstration of COupled models and their VALidation against Experiments. Decovalex III was the third phase of the DECOVALEX project series and operated through the period 1999 – 2003.

<sup>8</sup> The FEBEX project documentation uses "thermo-hydro-geochemical" (THG), but in this report the more common thermo-hydro-chemical (THC) and thermo-hydro-mechanical-chemical (THMC) are used. THmC denotes models where only limited mechanical couplings are included (typically to represent swelling e.g. Zheng et al. 2011).

THC/THmC modelling in the FEBEX I & II projects was performed using the UDC codes CORE<sup>2D</sup> V4 (Samper et al. 2003 and 2011), FADES-CORE (Juncosa 2001), INVERSE-CORE<sup>2D</sup> (Dai & Samper 2004), and INVERSE-FADES-CORE (Zheng & Samper 2004 and 2005). These numerical tools have been used to:

1. Interpret various laboratory tests for parameter estimation and to identify relevant geochemical processes.
2. Predict the transport patterns of artificial tracers added at both the Mock-up and In Situ Tests.
3. Predict the THC performance of the engineered barrier for the Mock-up and In Situ Tests.
4. Testing THC predictions against dismantling data from Heater # 1 of the In Situ Test.

These THC/THmC models of laboratory experiments, and Mock-up and In Situ Tests have been reported in Enresa (2000), Samper et al. (2005b), Enresa (2006a), Enresa (2006d), Samper et al. (2008a), Samper et al. (2008b), Zheng & Samper (2008), Zheng et al. (2008), Zheng et al. (2010) and Zheng et al. (2011).



## 2 Evolution of EBS and Geosphere 1997 – 2012

### 2.1 In Situ Test

The evolution of the In Situ Test has been considered in four phases:

- Excavation, construction and sealing: 01/07/96 – 27/02/97
- First operational phase: 27/02/97 – 28/02/02 (day 0 – 1'827)
- Excavation & recovery of Heater # 1 and resealing: 28/02/02 – 26/07/02 (day 1'827 – 1'975)
- Second operational phase: 26/07/02 – onwards (day 1'975 – onwards)

For the In Situ Test, day number is defined from 27/02/97 (day 0). In this report data have been considered up until 28/02/12 (day 5'478) corresponding to 15 years of continuous operation of the In Situ Test and slightly longer for the Mock-up. The evolution of the In Situ and Mock-up Tests during FEBEX I & II is described in Enresa (2006a). Detailed consideration of the sensor data has been provided during both experiments as a series of data reports. The conditions at the end of FEBEX II are described in Enresa (2006f, 2006g) and most recently, after approximately 15 years, in Martín & Barcala (2011) and AITEMIN (2012). A comparison of the two tests covering the first 13 years of saturation, together with additional information from laboratory testing is given in Villar et al. (2012).

Fig. 2-1 shows stress, temperature and relative humidity from Section F2 centred on Heater # 2 to day 5'478.

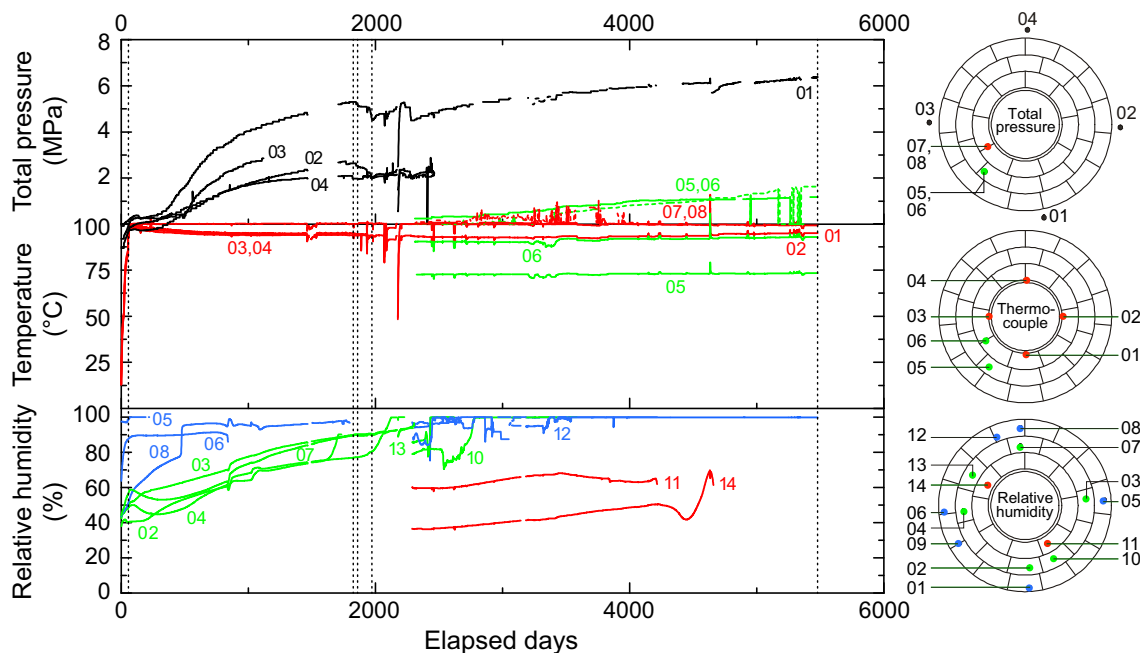


Fig. 2-1: Stress, temperature and relative humidity from "hot"<sup>9</sup> slice Section F2 (centre of Heater # 2).

Dashed vertical lines show changes in boundary conditions including switching off and removal of Heater # 1.

<sup>9</sup> "Hot" slices refer to vertical sections (for sensors or sampling) at one of the heaters. "Cold" slices are sections away from the heaters, i.e. at the mid-point between them or at the ends of the test section.

### **2.1.1 FEBEX I: Excavation, construction and sealing**

The construction of the FEBEX experiment was the first real-scale test of a horizontal disposal system for HLW. Some simplifications of the repository design were made with regard to the size of the bentonite blocks and the equipment and method of emplacement. After a test installation at AITEMIN's facilities in Toledo, emplacement procedures were refined to protect the blocks and to dry the working area in the drift to minimise the time that bentonite blocks were exposed to the GTS environment (close to 100 % humidity in summer). Construction was completed in 16 weeks between 01/07/96 and 15/10/96, two weeks ahead of schedule. Assembly and setting up of the data acquisition and control systems was not time-critical and was completed on 27/02/97.

The buffer was constructed manually. Sensors within the rock were emplaced before the buffer while sensors in the bentonite were installed in mechanically made holes within the blocks on completion of each slice. In all, a total of 136 slices were installed, made up of 5'331 blocks with an overall mass of 115.7 tonnes of bentonite. The average dry density was  $1.60 \text{ Mg/m}^3$  and the volume of construction gaps was 5.5 %. The design of the blocks and manufacturing tolerances resulted in a void of approximately 2 to 3 cm at the top of each vertical slice.

The heaters were of the same external dimensions and outer material as the canister in the AGP Granito concept: a carbon steel cylinder measuring 4.54 m, diameter 0.9 m and weight of ~ 11 tonnes (Enresa 2000). The heaters were transported along the tunnel and emplaced within a central steel liner of outer diameter 0.97 m using a transport and insertion car running on rails laid on the concrete sill of the tunnel. The alignment of the transport insertion car and the lower surface of the steel liner was the critical factor for successful emplacement (Enresa 2000).

The test zone was sealed with a keyed-type cast concrete plug designed to withstand a load equivalent to a swelling pressure of 5 MPa. The plug was constructed in 3 sections. The concrete was vibration-compacted but this did not give a complete seal around the key which was later filled by injection. Cable bundles were passed through the plug via four plastic pipes, which were then filled with mortar.

### **2.1.2 FEBEX I and II: First operational phase (5 years)**

The first operational phase was initiated by switching on the two heaters on 27/02/97 at a constant power. The temperature distribution quickly reached an approximate equilibrium after the switch to constant temperature control on day 61 (see Fig. 2-1). Temperature rose most quickly near the heaters. The temperature distribution in the buffer was approximately radially symmetric with axial variations according to position relative to the heaters. Temperatures are typically higher below the heater – probably due to the position of the heater within the steel liner. An ongoing slight decline in temperature on the steel liner surface was observed and temperature differences of up to 20 °C were measured along the surface of the heater. Temperature in the mid part of the buffer reached 50 – 60 °C and either stabilised or showed a slow increase. At the outer part of the buffer (rock-contact) temperatures rose more gradually to about 20 °C. A similar pattern of gradual temperature rise was observed in the rock with the magnitude decreasing with distance from the heaters (Enresa 2000).

After an initial adjustment of the vibrating wire parameters in the data acquisition unit, the measured total pressure increased with ongoing saturation. Highest values were at the rock/buffer contact and reached over 5 MPa. Loads on the liner were lower than ~ 2 MPa. In the rock, stresses showed a typical increase but the magnitude was highly dependent on location.

Within the bentonite buffer close to the rock, relative humidity quickly reached high levels indicating that the bentonite was close to saturation. There was good consistency between the different sensor types. Some sensors showed step-like changes while others showed a steady increase in relative humidity. Near the heaters, drying resulted in a sharp reduction in measured relative humidity over about the first year followed by a steady slow increase. The effect was largely controlled by distance from the heaters and was visible in the central part of the slice between the two heaters (Section H). Intermediate sensors showed a range of initial behaviours (rise/fall) but subsequently (after the first year) were typically slowly rising. It was also interesting that, in the sensors near the heaters, there was a temporary increase in relative humidity prior to the strong drying. This was due to a vapour front coming from the inner buffer and passing through the sensor region. This observation was reproduced by the coupled THM model (see Chapter 3). There was no indication of desaturation of the rock and both psychrometers and TDRs in the rock indicated an increase in water content from the initial condition (Enresa 2000).

Pore pressures typically stayed low relative to that in the geosphere (~ 1 MPa away from the open drift), although pressures reached 400 kPa at some sensors where saturation was high. Pore pressure in the radial boreholes typically showed ongoing recovery and there was no significant change in pressure for more distant borehole intervals.

Gas sampling started 3 months prior to the start of heating. Samples were analysed for hydrogen, methane, ethane, propane, butane, carbon dioxide, oxygen and nitrogen (Fernández et al. 2007). Samples indicated a reduction in oxygen content to around 1 – 2 % and ongoing hydrogen generation due to metal corrosion although this typically varied over time. Significant variations in oxygen content suggest that the bentonite barrier was not completely gas-tight.

During this phase water was leaking through the tubes containing the cable bundles<sup>10</sup>. Outflows ranged from 1 to 4 mL/min, with the majority believed to come from borehole SI-2. The total drift inflow (prior to drilling of instrumentation holes) had been previously estimated at 7.8 mL/min.

### **2.1.3 FEBEX II: Excavation, recovery of Heater # 1 and sealing**

Prior to the partial dismantling, Heater # 1 was switched off on 28/02/02 one month before starting the dismantling operations, so that the temperature in the area affected by the dismantling could be reduced to a level compatible with manual working (25 – 30 °C). The dismantling was carried out by AITEMIN causing a minimum disturbance in the section of the test corresponding to Heater # 2, which was in continuous operation. Data acquisition was maintained during the dismantling. In the sections around Heater # 1, an overall drop of temperature to around 25 °C occurred with the relative humidity near the heater increasing from 20 – 24 to 32 – 52 % just prior to dismantling as the temperature dropped and the convective flow of moisture due to the heater reduced. In the outermost part of the buffer the relative humidity slightly increased as a consequence of cooling (Enresa 2006a).

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<sup>10</sup> The design of the second concrete plug installed after partial dismantling in FEBEX II was effective in stopping this leakage.

The dismantling sequence was as follows:

1. Switching off Heater # 1, one month prior to plug demolition
2. Rock sampling in the service area
3. Demolition of the concrete plug (sampling)
4. Removal of bentonite up to the front of the Heater # 1 (sampling)
5. Extraction of Heater # 1
6. Removal of liner and bentonite buffer up to the target point (sampling)
7. Insertion of a one-metre dummy steel cylinder in the central hole
8. Installation of the first set of new instruments
9. Construction of the first section of the shotcrete plug
10. Installation of additional instruments in the buffer
11. Completion of the shotcrete plug to a total length of 3 m

The 1 m-long carbon steel dummy, designed to withstand a load of 8 MPa, was inserted into the central void within the liner left by the Heater # 1. Additional sensors were installed in the buffer prior to the construction of the first part of the new plug. Three new gas injection and collection pipes for sampling and permeability measurements were installed in the buffer in April 2003. The new plastic pipes with sintered stainless steel filters were inserted in boreholes drilled through the first part of the plug and into the buffer parallel to the drift axis, so that the long filter was centred on Heater # 2. Further sensors were also installed in plastic pipe extending to the centre of Heater # 2 (Section F2). A list of the additional sensors is given in Tab. 2-1.

Tab. 2-1: Additional In Situ Test sensors, installed during partial dismantling (Enresa 2006a).

Parameter	Sensor	Type	Plug/rock	Buffer	Total
Temperature	Thermo-couple	T	1	8	9
Total pressure	Vibrating wire	P	4	9	13
Relative humidity	Capacitative	WC		21	21
Plug displacement	LVDT <sup>11</sup>	SP	4		4
Gas flow	Manual	GF		6	6
Water sampling	Fibre	WS		18	18

<sup>11</sup> Linear variable differential transformer

A comprehensive sampling campaign was performed during the partial dismantling. The aims were (Enresa 2006a):

- to assess the behaviour and current state of the different elements in the In Situ Test after five years of heating and hydration, and to further understand the processes that took place within the buffer
- to evaluate the reliability of the data obtained from the instrumentation by calibrating the retrieved sensors, and to compare these data with the observations made from the samples taken
- to confirm the expected behaviour of the barrier under heating and hydraulic load
- to study the corrosion processes in the capsule, liner, purpose-made metal coupons and sensors

Samples were arranged in vertical sections labelled S0 to S31. S0 was located in the service area in front of the plug and S31 was located at 7.748 m into the EBS. A summary of the number and type of samples is given in Tab. 2-2.

Tab. 2-2: Number of samples taken during partial dismantling (Enresa 2006a).

Zone	Dismantling section	Rock	Concrete	Bentonite	Sensors	Metal	Total
Service area	S0	10					10
Plug	S1 – 7		56	15	23		94
Buffer	S8 – 31	23		623	141	6	793
Total		33	56	638	164	6	897

Post-mortem examinations and recalibrations of instruments were also performed. In general, sensors were in reasonable condition although the effects of bentonite expansion and corrosion were observed (Enresa 2006e).

Corrosion of the liner was generalised and non-uniform, with maximum values of 130  $\mu\text{m}$  (external) and 200  $\mu\text{m}$  (internal surface) with no evidence of localised corrosion (Fig. 2-2). There was no evidence of corrosion on the stainless steel or titanium coupons in the buffer, while carbon steel and copper coupons showed slight generalised corrosion with rates of  $\sim 0.1$ , and 0.71 (Cu-ETP) and 0.74 (CU10Ni)  $\mu\text{m}/\text{year}$  (Fig. 2-3). Only negligible corrosion was observed for Cu30Ni alloy (Enresa 2004a).

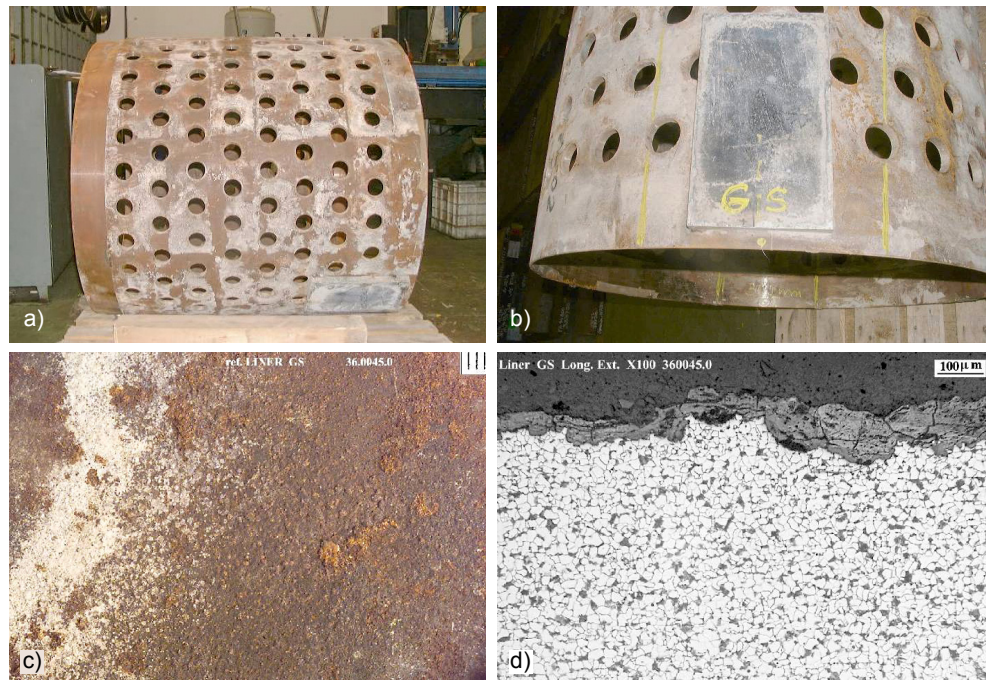


Fig. 2-2: Corrosion of the liner: a) Liner segment from dismantling, b) external surface of liner, c) detail of external surface and d) optical micrograph of external surface (Enresa 2004a).

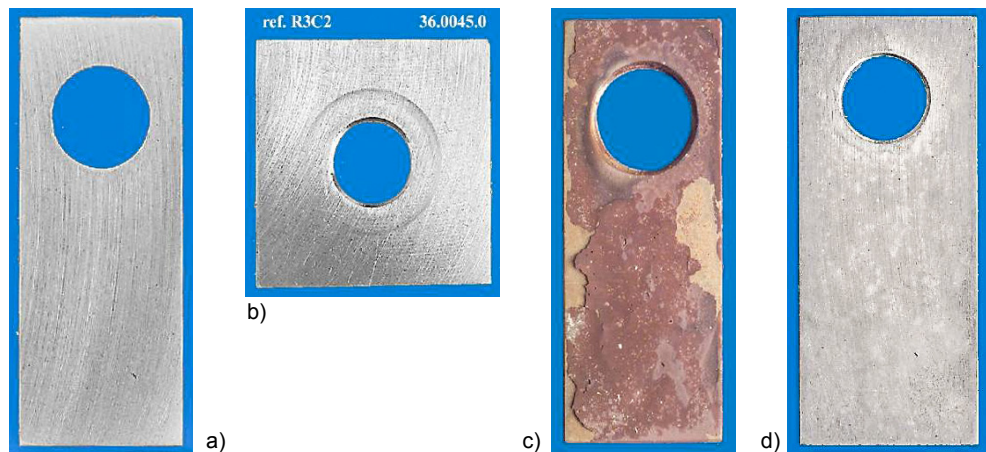


Fig. 2-3: Corrosion coupons after retrieval: a) Stainless steel (316L steel) coupon R2C2, b) Titanium (Ti GR2) R3C2, c) Copper (Cu-ETP) R4C2 and d) Copper (Cu30Ni) R4C5 (Enresa 2004a).

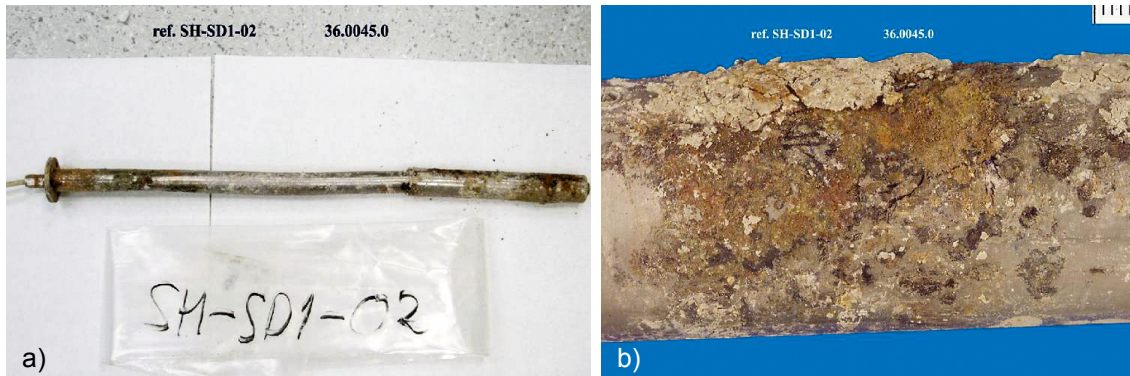


Fig. 2-4: Extensometer arm SH-SD1-O2 from instrument Section D1: a) extensometer arm after dismantling and b) detail of corrosion from location near liner (Enresa 2004a).

The highest corrosion effects were found at a highly instrumented section at the front of Heater # 1 (including extensometer SH-SD1-O2 shown in Fig. 2-4). Corrosion was due to the combination of sulphate-reducing bacteria and high humidity together with high stresses and the presence of chlorides (Fig. 2-4). Corrosion morphology suggested a localised phenomenon with cracking typical of stress corrosion in the presence of chlorides. Microbial analysis indicated the presence of aerobic and sulphate-reducing bacteria in the bentonite around this instrument section but not in a sample from another section (Enresa 2004a). The concrete plug was not specified for either water or gas tightness, so it is likely that air could pass through the plug (it has been suggested that hydrogen concentrations reduced during the early part of the test due to escape through the plug, Enresa 2000). In addition, pipes passed through the plug for instrumentation and gas sampling. These pipes were open into the bentonite via steel filters although some pipes were water filled in the bentonite near the rock contact. The high density of sensors may have facilitated water vapour transport in this area.

The bentonite sampling and analyses are documented in Enresa (2006b) and the discussion below is largely taken from there. Additional discussion is presented in Villar et al. (2005) and Villar & Lloret (2007).

- The distribution of water content and dry density was axially symmetric with similar average values in the sections studied. Sections around the heater showed a higher water content gradient (see Fig. 2-5, Fig. 2-6). Average water saturation was 85 %. Dry density was highest near the heater and lower at the host rock contact.
- Dry density decreased to 1.58 Mg/m<sup>3</sup> from the compacted block density of 1.70 Mg/m<sup>3</sup> due to the filling of construction gaps. This density is slightly below that estimated at construction.
- There was no influence from geological structures and water content showed strong radial symmetry regardless of the presence of water-bearing fractures (the transmissive lamprophyre structure intersects the drift at Heater # 1; see Fig. 2-7).
- There is good agreement between measurements of water content and the relative humidity from sensors.

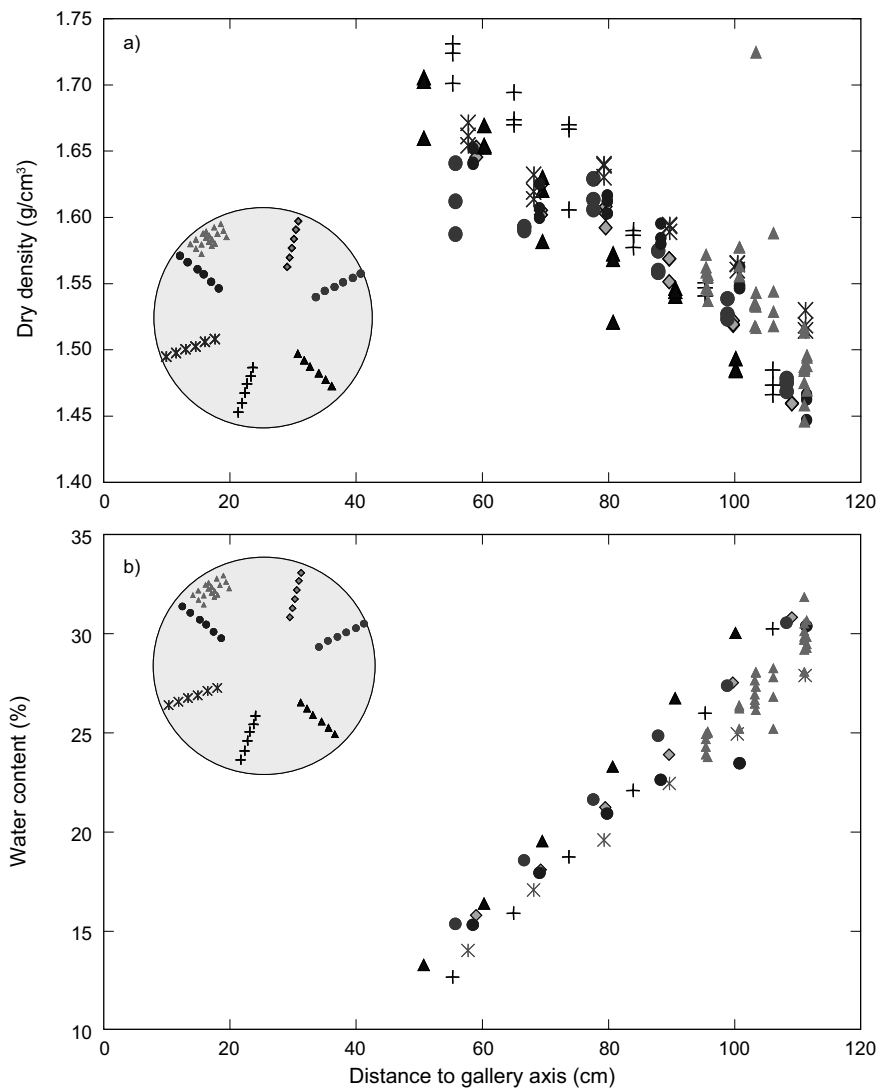
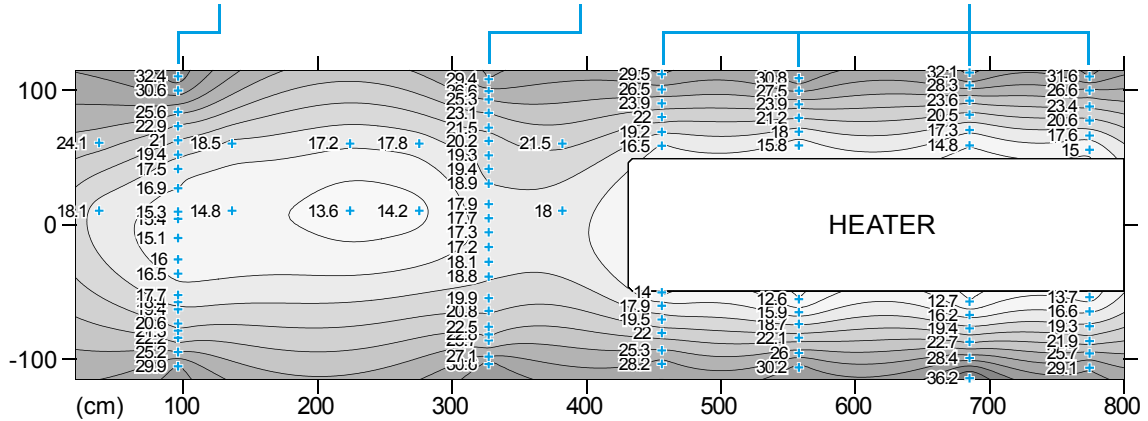
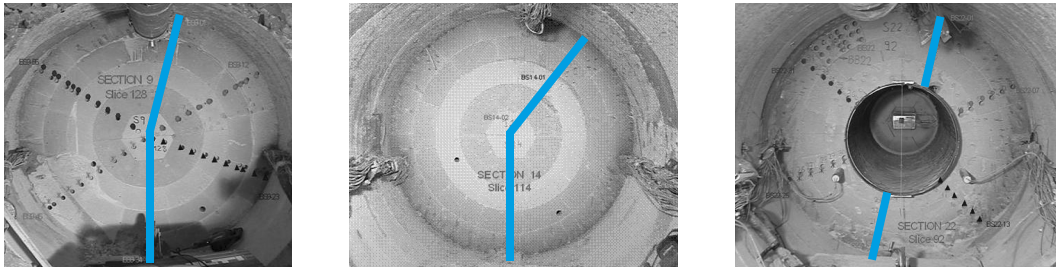
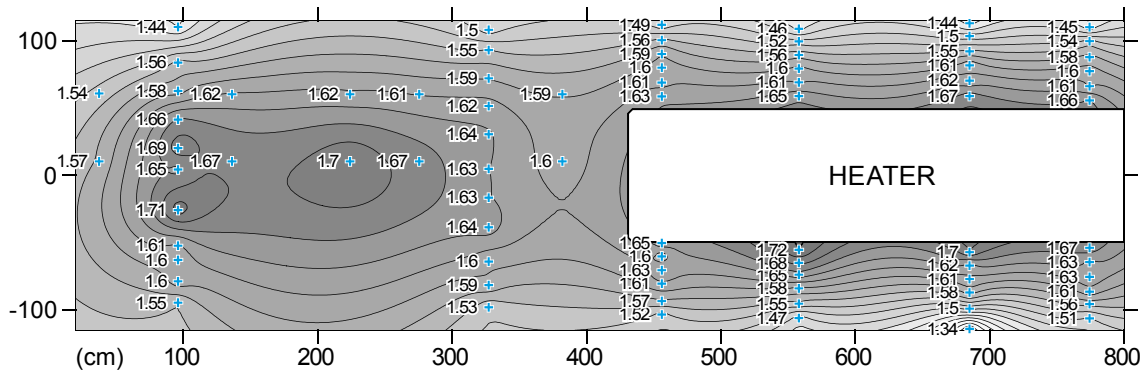


Fig. 2-5: Water content and dry density distribution determined in specimens recovered from a section around Heater # 1 (from Villar et al. 2005).

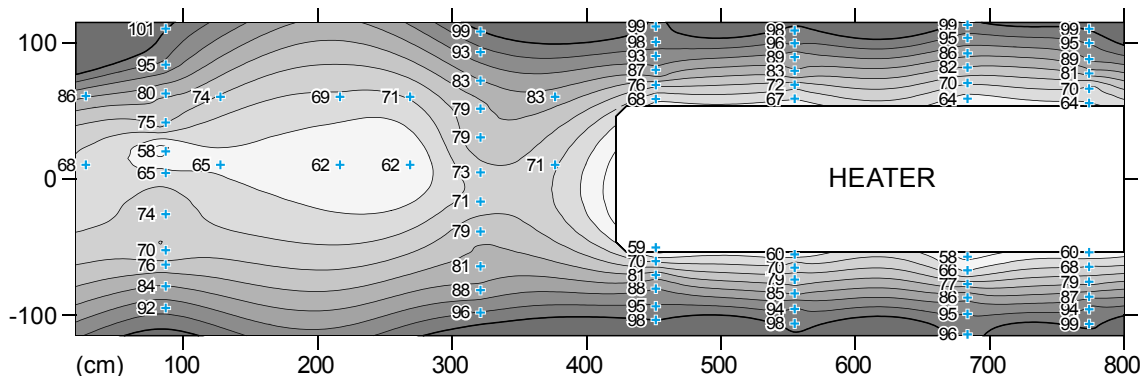
a) Sampling sections



b) Water content (%)



c) Dry density (g/cm³)



d) Degree of saturation (%)

Fig. 2-6: Sampling sections (a) and longitudinal distribution along the gallery of water content (b), dry density (c) and degree of saturation (d).

From Enresa (2006b).

Mineralogical and geochemical characterisation suggested that no great changes occurred in the bentonite during the five years of saturation and heating. At a macroscopic scale, no mineralogical change could be identified (Enresa 2006b). However, at a microscopic level, signs of dissolution and re-precipitation of potassic feldspars were identified in the sample in contact with the heater. The feldspars showed dissolution crevices with nearby neo-formed minerals and clay minerals with filament-like morphology. Similar changes were visible in laboratory tests (Fernández & Villar 2010). In addition, the following chemical changes in the buffer were observed (Enresa 2006b).

- The cationic exchange capacity increased with respect to the initial state, due mainly to the overall increase of exchangeable potassium and calcium. Analyses by CIEMAT and INPL (l'Institut National Polytechnique de Lorraine) showed a consistent increase from  $\sim 100$  meq/100 g to 103 – 105 meq/100 g. An increase of exchangeable sodium (and probably of magnesium) was observed towards the granite in sections with a range of thermal gradients. In the case of calcium, there was an increase in its content at the heater contact and at the bentonite – granite contact.
- Hydration of bentonite at the external blocks in contact with the granite produced the dissolution and dilution of the more soluble trace minerals in the bentonite (sulphates, carbonates and chlorides) that were transported towards the inner part of the barrier. As a result, saline fronts were generated due to the different mobility of the dissolved ions: the tendency of Na, Ca and Mg concentrations was similar to that of chloride, while sulphate mobilisation was significantly retarded with respect to chloride. Temperature seems to have a significant influence on salt movement: salt movement was faster in the heater section than in the colder zone. As a result, chloride content increased considerably towards the hot zones (Enresa 2006b). Similar processes have been observed in tests on compacted bentonite performed in cylindrical cells with thermal and hydraulic gradients (Fernández & Villar 2010).
- The chemical and mineralogical composition of the bentonite from dismantling Section S7 (see Tab. 2-2) in contact with the cement plug is rather similar to that of the as-compacted bentonite, except for an increase in the aluminium content and for the local occurrence of higher quantities of calcite and gypsum. There was also an increase of Ca, Na and K in the exchange positions and an increase in salinity of the porewater. The section was one of the coldest so reactivity may have been limited.

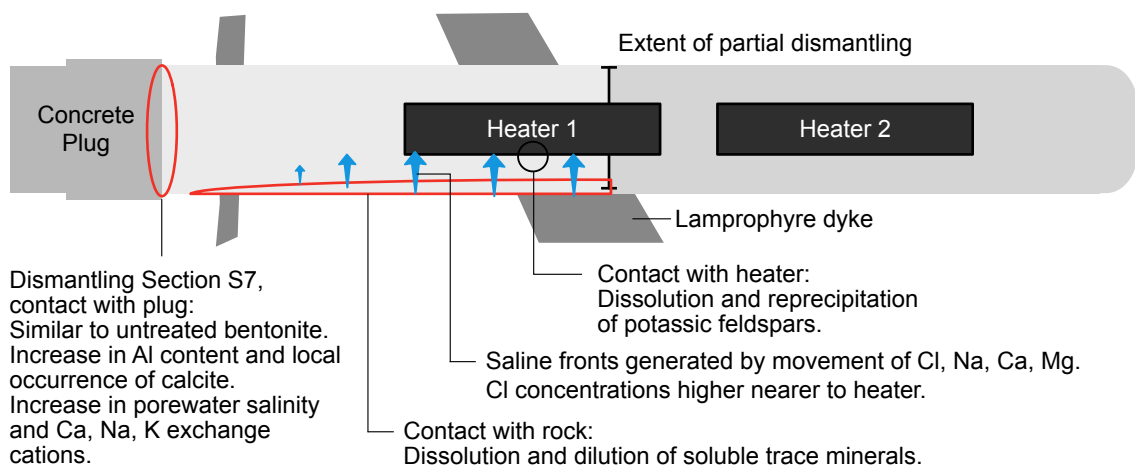


Fig. 2-7: Schematic showing locations where indications of mineralogical and geochemical changes were observed.

The THM behaviour of the recovered bentonite was compared with that of untreated FEBEX bentonite (for further discussion see Enresa 2006b, Villar et al. 2005, Villar & Lloret 2007). The results obtained indicated:

- No significant change in water retention capacity, hydraulic conductivity or swelling capacity as a function of dry density. Variations in the values obtained were mainly related to dry density.
- The estimated preconsolidation pressures were lower than 10 MPa, which was a decrease from the initial preconsolidation pressure of around 40 MPa. Microstructural changes experienced during hydration are believed to account for this.
- A possible reduction in uniaxial strength of the bentonite for the samples that were subjected to higher temperature. There was a clear trend of reduction as temperature increased. The lowest uniaxial strengths were measured for two samples exposed to over 70 °C (Enresa 2006b) and were below reference values accounting for compaction direction. Values were however strongly dependent on water content.
- A possible decrease of up to 10 % in thermal conductivity (relative to an empirical relationship for untreated samples) for samples closest to the heater (Villar & Lloret 2007).

Overall, slight changes observed in the chemical and mineralogical composition of the bentonite cannot be clearly correlated with any significant variation in the macroscopic thermo-hydro-mechanical properties. There is a possible increase in plasticity of the samples from the outer ring that could be linked to the increase in exchangeable sodium that took place near the gallery wall, which would also be responsible for the tendency of these samples to form colloids.

Temperatures around Heater # 2 and the end of the tunnel were relatively unaffected by the dismantling operations. Total pressure declined during dismantling but recovered over the next 1'000 days with a generally increasing trend.

#### **2.1.4 FEBEX II, NF-PRO and FEBEXe: Second operational phase (10 years)**

The start of the second operational phase is defined as 26/07/02 (day 1'975) corresponding to the end of construction of the first part of the shotcrete plug. After disconnection of Heater # 1 it was necessary to increase power to Heater # 2 by approximately 5 % to compensate for the loss of output from Heater # 1. The heater power requirement has continued to increase since then, probably due to increasing thermal conductivity of the bentonite as saturation increases. In a repository system power output from the waste canisters would fall exponentially over time with temperatures in buffer and rock returning close to the undisturbed value within 1'000 years (e.g. Hökmark et al. 2009, 2010).

In the In Situ Test after an initial transient phase, where conditions between the plug and the face of Heater # 2 equilibrated to the new boundary conditions, temperature in the buffer and rock quickly stabilised.

Relative humidity (RH) in the buffer resumed a slow increase in all but the outer ring of the buffer, which was already highly saturated. By the end of the 15 years, relative humidity in the intermediate ring was also high (100 %) and sensors in the inner ring around the dummy canister showed high relative humidity ~ 90 %. Around the heater, one sensor shows 100 % RH while another shows ~ 60 % RH. These values were either stable or slightly declining over the last year. Within the rock, there was some evidence of desaturation related to the excavation of Heater # 1 but otherwise a slow increasing trend in relative humidity was observed.

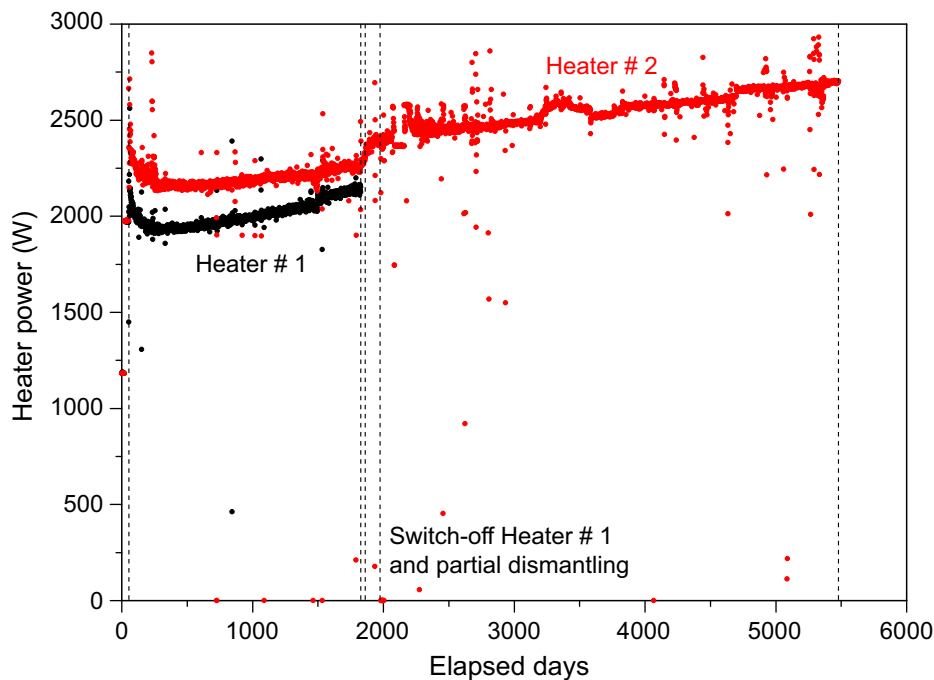


Fig. 2-8: Power output from Heater # 1 and # 2 (note increase after switch-off of Heater # 1).

Total pressure rose throughout the buffer during the period, although several sensors became inoperative. A maximum stress of 6.4 MPa was observed on the rock wall at Section F2. In the same section closer to the heater, stresses were typically lower and tangential (hoop) stress has, since about day 4'900, exceeded radial stress (see Fig. 2-1). This is the only total pressure sensor pair still operating in the buffer. Stresses at the bentonite/heater contact are uncertain due to the lack of working instruments, although a stress of over 3 MPa was measured at Section E2 prior to sensor failure in 2005.

Pore pressures have shown a general increase since the start of the phase, although individual sensors show both rises and falls over periods of hundreds of days. There is no clear evidence of a consistent ongoing rise in pressure and AITEMIN (2012) report that pore pressures may have stabilised.

Gas and porewater sampling were performed within the FEBEX II and NF-PRO projects (Fernández et al. 2007) although water sampling was limited by the low permeability of the buffer.

### 2.1.5 State of In Situ Test after 15 years

The FEBEX In Situ Test was running for over 15 years and was still in good operational condition. Measurements from sensors in the EBS and geosphere showed either near constant behaviour or very slow trends as listed in Tab. 2-3. Temperature was stable, heater power and total stresses were increasing slowly within the buffer (50 – 150 kPa over the last year) indicating ongoing saturation although there was evidence for some stabilisation in relative humidity close to the heater. Humidity sensors in the inner ring even showed a recent slight reduction. Pore pressures had developed in the outer parts of the buffer but it is difficult to determine whether they had stabilised or would have continued to slowly rise.

Over the last few years of operation the sensors continued to operate well under the current maintenance regime with no sensor failures in the last two years. High rates of sensor failure had in the past been associated with the dismantling of Heater # 1 and installation of cable boxes to make the pathway watertight in the new plug. While there was still considerable temperature information, the coverage of the relative humidity and total pressure datasets had reduced. In particular, only a limited number of total pressure cells were still operative and further failures would have limited the usefulness of the dataset.

The constant temperature control (100 °C – the design temperature for the disposal reference concept) applied at the heater surfaces resulted in an increasing power input to the heater as the thermal conductivity of the bentonite increased. This is contrary to the behaviour expected in a HLW repository where temperature would peak within the first decades and gradually decline after that as the power output of the fuel declines<sup>12</sup>.

Tab. 2-3: FEBEX sensor trends during the 15<sup>th</sup> year of operation (taken from AITEMIN 2012).

Property/sensor	Trend over 15 <sup>th</sup> year of operation
Temperature	Trends are maintained with a general very slow increase. Temperatures in the bottom part of the drift are higher than in the sides and upper part (temperatures are higher in the base of the liner).
Geosphere pressure	Some recent falls in pressure. Radial boreholes: practically stabilised although some decrease in pressure.
Bentonite pore pressure	Pore pressures seem to have stabilised.
Relative humidity Capacitive sensors	Outer and intermediate rings of bentonite blocks show 100 % RH. Inner ring is close to saturation in the contact with the dummy canister, with values over 92 %, although lately showing a very slight decrease.
Relative humidity TDR sensors	In the bentonite: recent slow decrease starting in the external and intermediate rings, while rising at constant rate in inner ring . In the granite: in Section M1 around the plug, water content seems to be increasing very slowly.
Psychrometers	No changes are observed lately by the sensors still in operation.
Total pressure	In general total pressure continues to increase at all points in the buffer, and at the bentonite/rock contact, with the exception of Section G.
Displacements	Concrete plug: practically no variation. Heater: poor confidence in sensor readings. Bentonite blocks and rock extensometers: almost constant.

<sup>12</sup> The choice of constant temperature control was made to save time in the initial heating phase of the experiment.

## 2.2 Mock-up test

The Mock-up was constructed within a specially designed annex at CIEMAT. The steel confining structure was lined with four layers of geotextile (total thickness 6 mm). The bentonite blocks were then emplaced one vertical slice at a time from the central slices (between the heaters) outward. The heaters were then mechanically inserted into horizontal holes in the block array. Sensors were installed in holes machined into the bentonite blocks. Tracers (filter papers, sintered metal capsules and compacted bentonite pellets) and metal specimens for corrosion studies were also inserted. Three days prior to the start of the test, 634 litres of water were injected at a rate of 3.5 L/min to fill the voids between the blocks. Since then, water pressure has been maintained at 5 – 6 bar (nominal 5.5 bar). The rate of injection follows a steep decline reducing to an average value of 0.03 kg/day over the last year (10.9 kg/a).

### 2.2.1 Evolution of EBS 1997 – 2012

Operation of the Mock-up started on 04/02/97 at 12:45 with the switching-on of the heaters. The heater power was raised in stages over the first 10 days until the heater surface temperature achieved 100 °C. After this, a roughly constant temperature was maintained, with the exception of minor power interruptions and the overheating period (26/11/00 – 28/11/00).

During the overheating incident, due to a failure in the heating control system, temperatures near the heaters rose to more than 200 °C. This overheating was halted automatically, but the temperature within the bentonite reached a maximum of ~ 240 °C at the control section (Enresa 2006g). The bentonite around the heaters dried and a thermal pulse was generated, followed by a cooling period. Normal surface temperatures were achieved by 04/12/00 (day 1'398). The effect of the overheating was studied by Cañamón et al. (2004), who found that there was no evidence for any "important consequences or irreversible perturbations of the processes or the sensors". Gens (pers. comm.) suggests that while the relative humidity has largely recovered it is possible that there may have been some ongoing disturbance to the measured stresses.

Problems with isolation of the heater resistances led to an interruption in the heating (23/06/02, day 1'965) and a subsequent switch to constant power on 03/07/02. Since then the temperature at the heaters' surface has remained slightly below 100 °C and the system shows some influence of the laboratory conditions with heater surface temperatures varying between 93 and 100 °C.

### Temperature in the Mock-up

After a very short initial transient related to heating lasting ~ 25 days, temperature throughout the buffer remains steady with a strong radial dependence related to distance from the heater and a slight warming trend. Superimposed on the trend are variations due to the applied heater power and external boundary conditions. Since the switch to constant heater power, a roughly annual oscillation (related to laboratory temperature) is visible with variations of 5 – 10 °C (Fig. 2-9).

Temperature data show a strong symmetry about the centre line (Fig. 2-10) and high reliability. Only at radius 1 on the B1/A1 slices there is evidence of an observable deviation from the general symmetric pattern controlled by distance from the heaters and the boundaries (sensors at radius 1 in Slice B5 and A4 show an offset but with an almost identical trend).

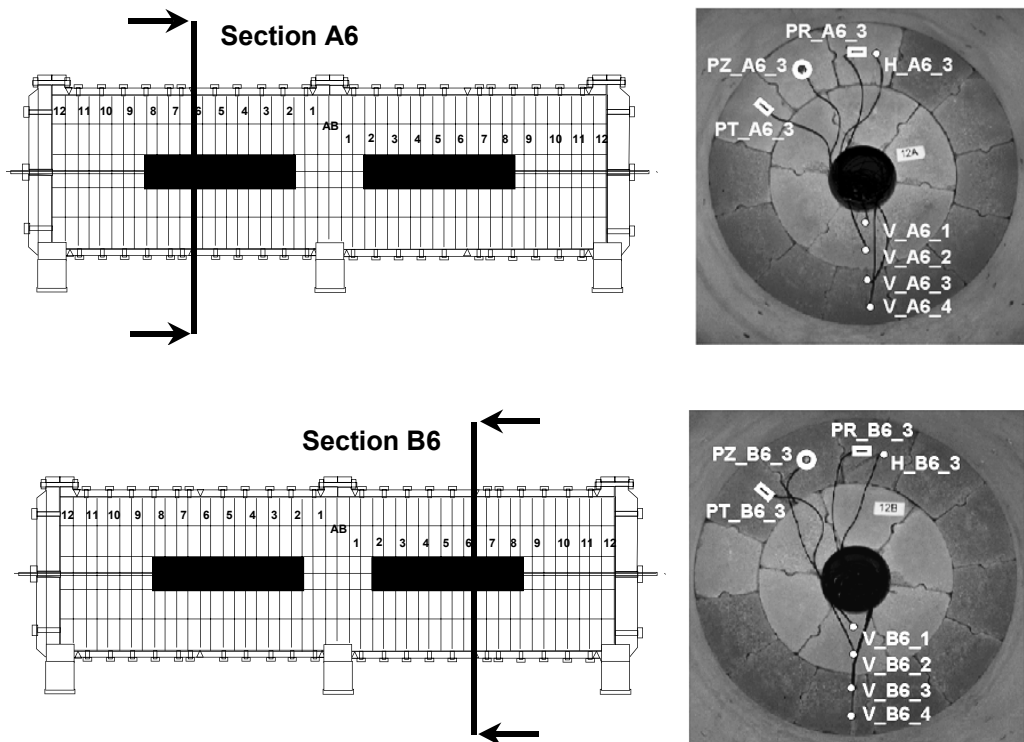
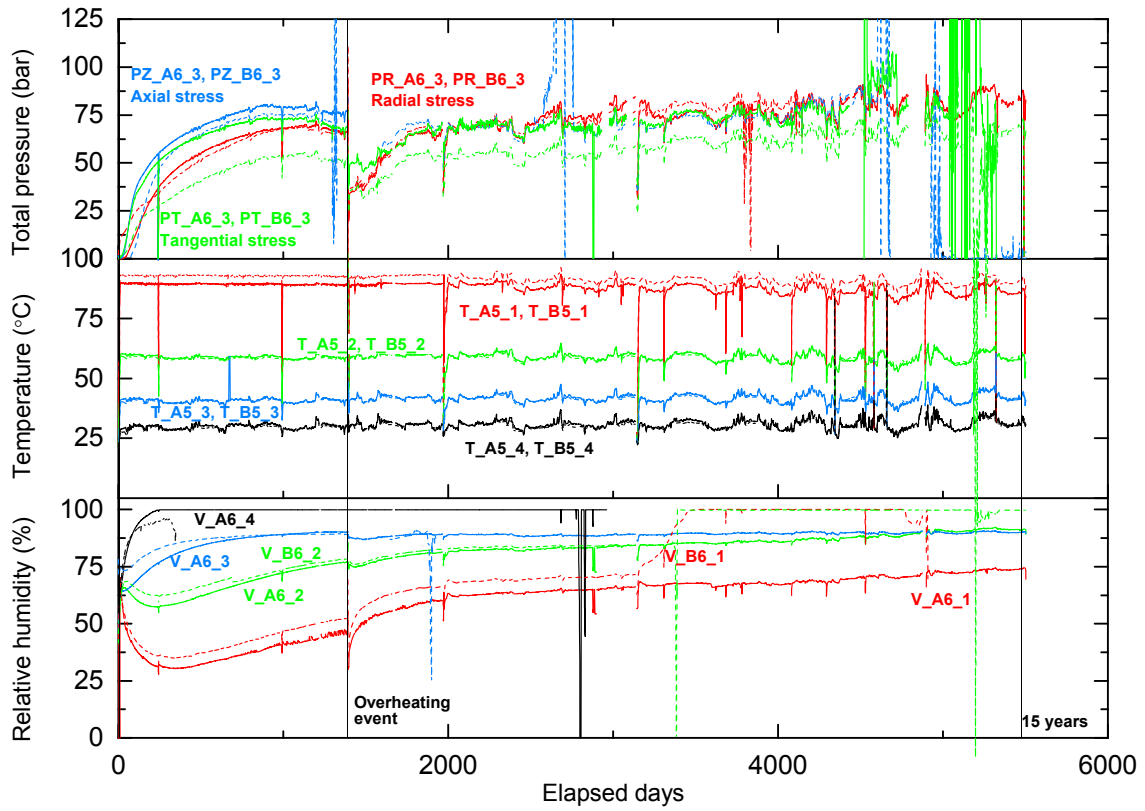


Fig. 2-9: Stress, temperature and relative humidity from "hot" Slices A6 (solid lines) and B6 (dashed lines).

The strong symmetry between the two slices is clearly seen. Oscillations in temperature and total pressure relate to seasonal variation in laboratory temperature.

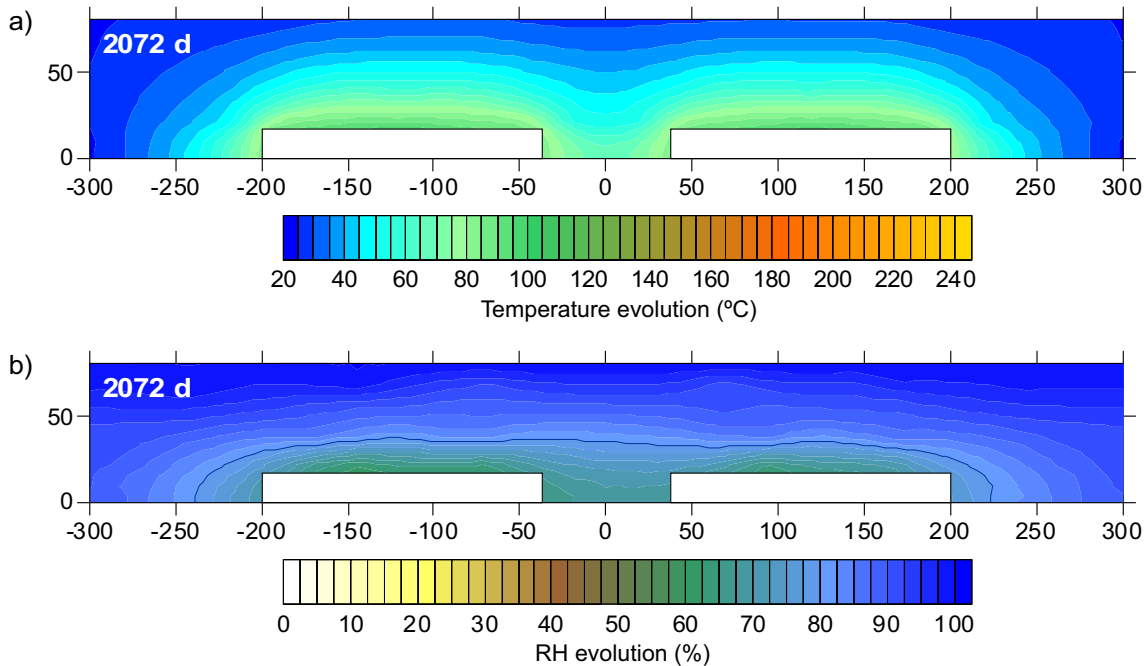


Fig. 2-10: a) Temperature and b) relative humidity contours from day 2'072 (Martín et al. 2006).

Axis labels show position in cm.

### Stresses in the Mock-up

Axial stresses ( $\sigma_{zz}$ ) rose quickly over the first 500 days before either stabilising or settling to a slow linear increasing trend. Axial stresses at radius 2 have risen more slowly than those at radius 3, but are now comparable in magnitude. In some locations measured axial stress is in excess of 10 MPa. Radial stresses also rose relatively quickly over the first 500 days. Radial stresses at radius 2 have risen more slowly than those at radius 3, with the exception of Slice AB where the sensor PR\_AB\_2 shows a significantly higher stress than PR\_AB\_3. The maximum stress measured is at sensor PR\_AB\_2 with a radial stress of  $\sim 12$  MPa (corresponding to the expected swelling pressure for the effective dry density of the core blocks of  $1.71 \text{ Mg/m}^3$ ). Tangential stresses at radius 3 rose quickly (particularly on the AB symmetry slice, where the respective sensors are located on the block joints - potential preferential hydration pathways and closer to the hydration surface) compared to those at radius 2, which showed a much more gradual rise in stress over several thousand days. At the AB slice, the radius 2 tangential stress rose above that at radius 3 after 1'500 days while for other slices the radial stress slowly approached that of radius 3 (e.g. Slice A3 & 4, A6 & 7, B3 & 4, B6 & 7).

Comparison of the stresses at locations where all three components are measured shows the development of a significant stress anisotropy which reduces over time, eventually resulting in (where measured) approximately isotropic conditions (see Fig. 2-9).

### Water content/relative humidity

After an initial transient period of  $\sim 500$  days, when moisture was redistributed in the buffer moving away from the heater towards the outer boundary, an overall increasing trend was established throughout the buffer (see Fig. 2-9). The relative humidity values near the outer

boundary (radius 4) are close to 100 % and relative humidity at radii 1, 2 and 3 is slowly increasing, however the rate of increase has reduced with time. Again a strong symmetry in relative humidity has been observed as shown in Fig. 2-10. The gradient between radius 2 and 3 flattens over time and can no longer be identified from relative humidity measurements after 4'500 days. Ongoing sensor saturation and failure (especially in the B-slices) make interpretation less certain but near steady-state conditions seem to apply in radii 2 – 4. At radius 1 relative humidity appears still to be increasing slowly.

### **2.2.2 State of the Mock-up Test after 15 years**

In summary, the experiment continues to run in good order, well beyond its original design life of 3 years. More than 85 % of the sensors remain operative and the heaters are working well at constant power (Martín & Barcala 2011). Recent changes in the control systems of the heaters are expected to extend working life. A near steady-state temperature distribution exists within the Mock-up perturbed by small annual variations together with some longer-term variability (total range  $\sim 10$  °C) caused by fluctuations in laboratory conditions. These quasi-steady-state thermal conditions have existed for several years. The variations in temperature are also evident in the total pressure data. Fluid pressures have increased over time with a rising trend emerging after 2'500 days in the cooler parts of the setup. Stresses of over 12 MPa have evolved within the buffer and may still be increasing although this is difficult to assess given the annual cycle.

Water inflow to the Mock-up shows a roughly log-linear decline over the 15-year period with initial rates of  $\sim 10$  kg/day down to an average of less than 0.02 kg/day in the last year as shown in Fig. 2-11. The total volume of water injected (as of December 2011) was 1'138 kg (equivalent to approximately 21.9 % water content).

Over the year to March 2012, the total water inflow to the experiment has been 10.9 kg equivalent to 0.2 % water content. Assuming that inflow remains constant (despite the observed decline) a hypothetical further 15 years of operation might therefore result in an increase of about 164 kg or 3 % water content.

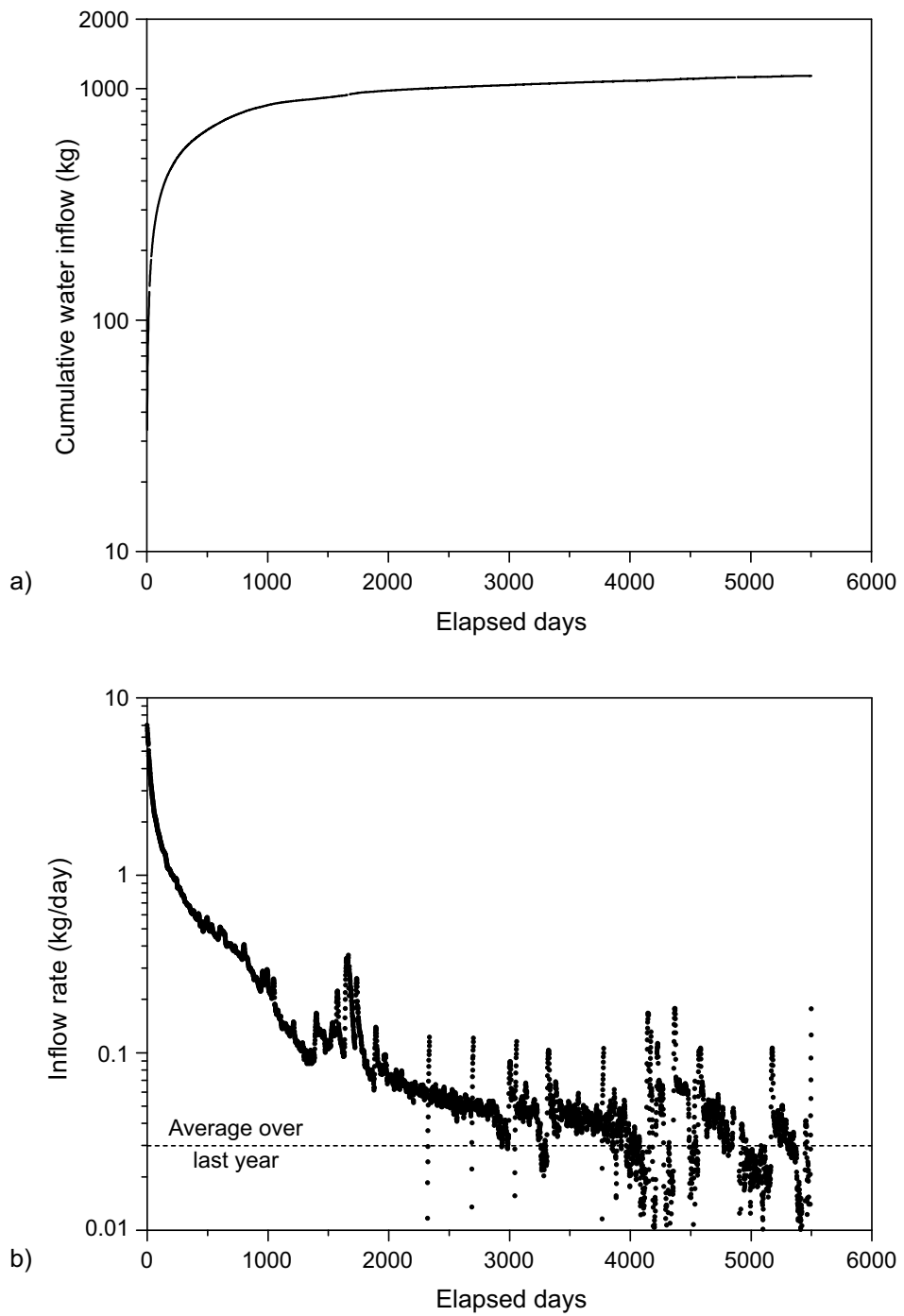


Fig. 2-11: Water inlet, a) cumulative total (kg) and b) estimated inflow (30-day least-square fit).

Dashed line shows fitted slope over last year of 0.02 kg/day.

### 2.3 Comparison of In Situ Test and Mock-up Test evolution

Geometry and material property differences between the In Situ and Mock-up Tests (see Section 1.4) hinder quantitative comparison between instrument responses in the two tests. However, to facilitate comparison, we have defined two locations at normalised radii  $r_n$ ,  $r_b$  to reflect the different locations within the buffer, relative to the system boundary conditions (heater and rock or geotextile). The selected sections are given in Tab. 2-4 and the radii have been defined as:

$$r_n = \frac{r}{r_{outer}}, r_b = \frac{(r-r_{inner})}{(r_{outer}-r_{inner})}$$

where  $r$  is the instrument radius (m);  $r_{inner}$  is the inner radius of the bentonite (In Situ Test liner or Mock-up heater radius) and  $r_{outer}$  is the outer radius. The normalised radii give the fraction of bentonite between the sensor and a) the centre of the test or b) the heater. So  $r_n$  or  $r_b = 1$  corresponds to the outside of the buffer,  $r_n = 0$  is the centre of the test (only relevant for sections without heater) and  $r_b = 0$  is the surface of the liner/heater. Fig. 2-12 shows the temperature evolution in the In Situ and Mock-up Tests for hot Sections F2 and A5, B5. The radial distribution of temperature sensors is limited in F2 although temperatures sensors from total pressure and relative humidity sensors can supplement the thermocouple data.

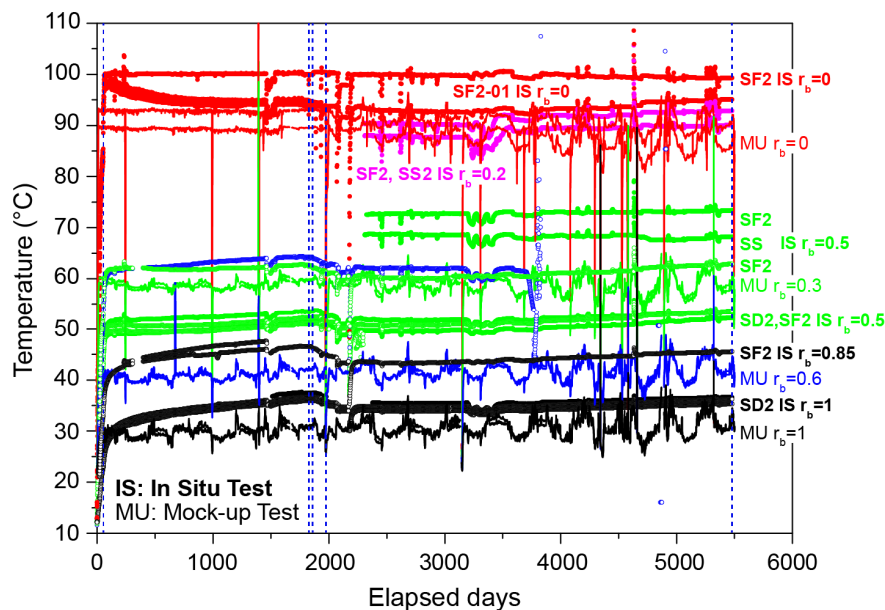


Fig. 2-12: Temperature from In Situ Test and Mock-up for hot Sections F2 with additional data from sensors in Sections S and D2 (In Situ) and Sections A5, B5 (Mock-up).

The data show that although boundary temperatures ( $r_b = 0, 1$ ) differ by only a few °C, the radial distribution of temperature is somewhat different due to the different ratio of buffer to heater radius and other influences<sup>13</sup>. The Mock-up test shows a strong temperature cycling due to the outer temperature boundary condition. The differences in temperature distribution are likely to influence the extent of moisture redistribution (drying/wetting) within the buffer and hence other parameters.

<sup>13</sup> A logarithmic distribution of temperature would be expected for steady heat flow in a uniform medium and might be the basis for future comparison of the two tests.

Tab. 2-4: Selected instrument sections (see Fig. 1-5 and Fig. 1-7) from In Situ and Mock-up Tests.

Section	In Situ	Mock-up
Hot/Mid-heater	F1, F2	A4 – 6, B4 – 6
Between heaters	H (up to dismantling)	AB
Cold	B1, B2	A10 – 12, B10 – 12

Fig. 2-13 shows a comparison of data from relative humidity sensors. Values are typically higher and more consistent in the Mock-up than in the In Situ Test. In the hot sections, outer radii saturate faster in both tests and inner radii show a characteristic desaturation in the first year prior to a slower saturation. In the centre sections (mid-way between heaters), similar trends are observed in the two tests but the desaturation is greater in the In Situ Test and saturations are typically lower. There is no relative humidity data from the cold sections of the In Situ Test.

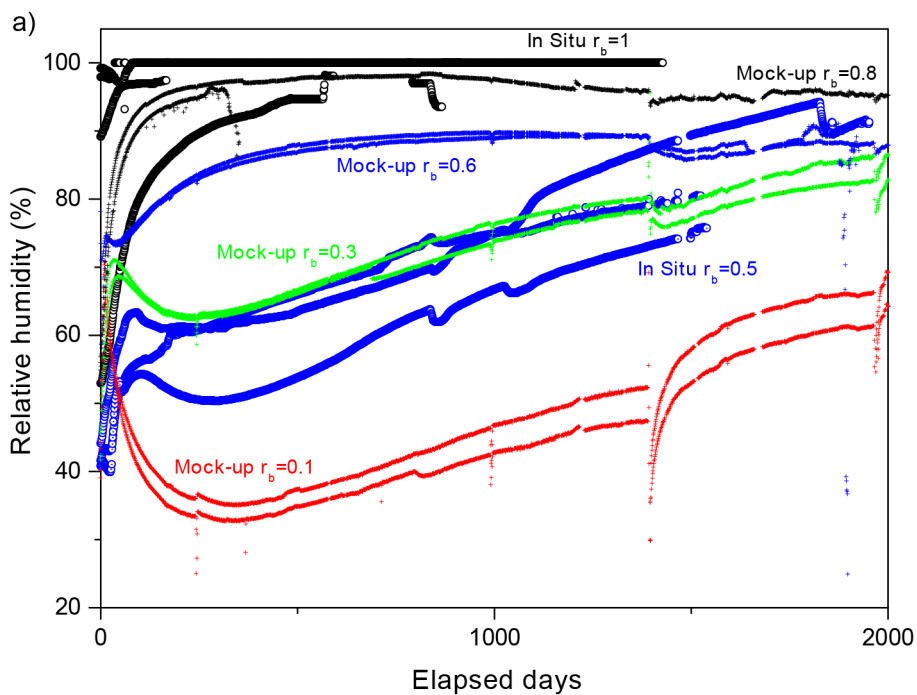


Fig. 2-13: Relative humidity of In Situ Test and Mock-up, a) hot Sections F1/B4,B6, b) hot Sections F2/B4,B6 and c) section mid-way between heaters H/AB.

Sensors in Section F1 removed during partial dismantling.

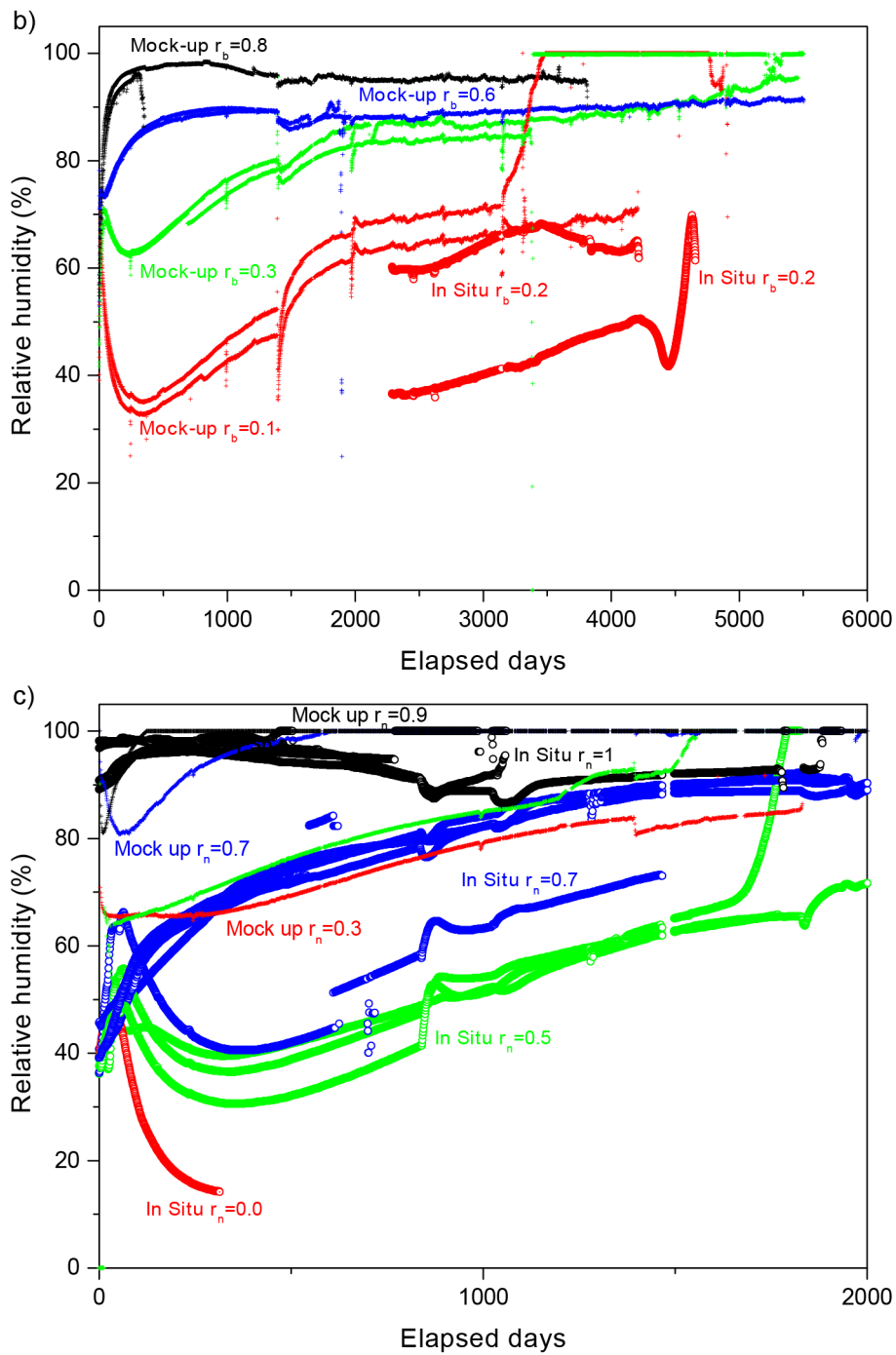


Fig. 2-13: (continued) Relative humidity of In Situ Test and Mock-up, a) hot sections F1/B4,B6, b) hot sections F2/B4,B6 and c) section mid-way between heaters H/AB.

Sensors in Section F1 removed during partial dismantling.

Fig. 2-14 shows a comparison of data from the total pressure cells. Stresses measured in the In Situ Test typically develop more slowly than in the Mock-up. Stresses are also relatively lower (even after consideration of the different expected swelling pressures – see Tab. 1-6) and show a clear ongoing upward trend.

The responses observed in the two tests are not incompatible. However, differences in dimensions and boundary conditions do not allow direct comparison. This lack of direct comparison between the two tests means that any demonstration of consistency in the observed responses largely rests on modelling using a common description of the buffer as described in the next section.

Higher initial saturations and stresses in the Mock-up relate to the flooding, where 634 litres of water were injected within three hours before the start of heating. Subsequently, 1'138 kg of water has been injected in the 15 years since the start of heating.

Over the 15 years, a clear slowing in saturation in the Mock-up has been observed. This is most strongly seen in the water uptake history in Fig. 2-11 (the water uptake for the In Situ Test is unknown). The slowing is also visible in the relative humidity and stress but is somewhat obscured by the annual temperature trend.

The cause of the slowing is uncertain. Initial investigations considered clogging of the geotextile or water injection nozzles, but these causes were discounted (see Appendix B for a detailed discussion) and subsequent investigations have concentrated on the behaviour of the bentonite and the influence of coupled processes (see next chapter).

The evidence for a comparable slowing in the In Situ Test is less clear (Enresa 2006c) and there are indications in the continuing increase in measured total pressure that the phenomenon is limited to the Mock-up (or at least less significant in the In Situ Test perhaps due to the lower dry density).

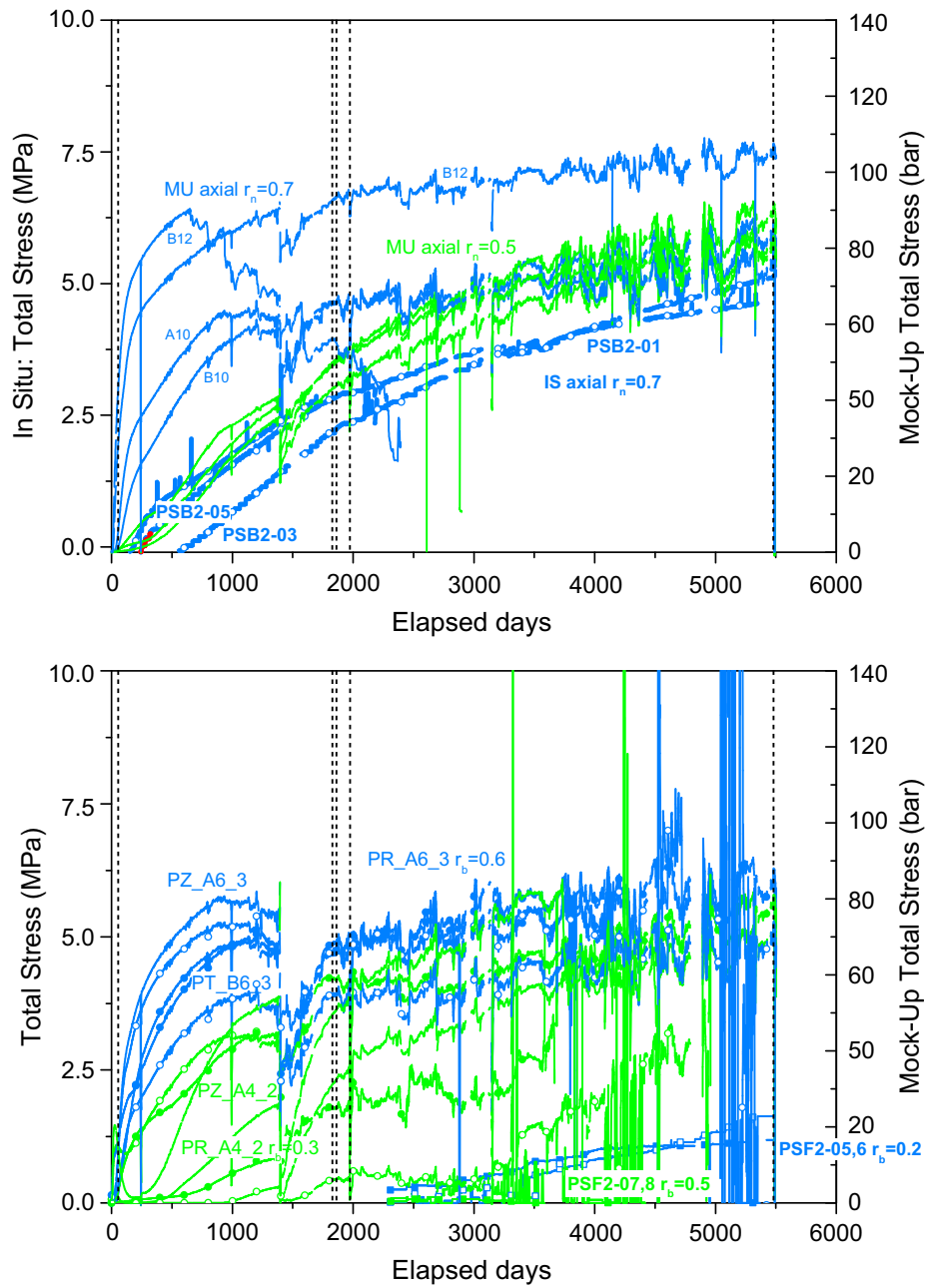


Fig. 2-14: Total pressure for the In Situ Test and the Mock-up, a) cold section, b) hot section. Vertical axes adjusted for expected swelling pressure difference (In Situ Test: 5.8 MPa, Mock-up: 8.2 MPa).



### 3 Modelling

The models discussed here all have the purpose of either predicting or interpreting conditions within the bentonite buffer (and for the in Situ Test, the near-field geosphere response) during the transient heating phase of the experiments. A summary of key modelling references for the In Situ Test and Mock-up is given in Appendix A.

#### 3.1 Conceptual models

##### 3.1.1 Thermo-hydro-mechanical models

The major processes occurring within the buffer have been identified by Gens et al. (2009) as:

- Thermal:
  - Heat conduction and advection<sup>14</sup> (mobile phases)
  - Latent heat of phase changes
- Hydraulic:
  - Liquid and gas flow
  - Water evaporation and condensation
  - Binary diffusion of air and water
  - Dissolution of air in water
  - Diffusion of air in water
- Mechanical:
  - Deformation due to changes in stress, suction, pore pressure & temperature
  - Deformation of both solid skeleton and constituent phases

Fig. 3-1 shows the major fluxes of the different phases in the buffer and the host rock adapted from Gens et al. (2009). Desaturation of the host rock is not thought to occur in the FEBEX In Situ Test due to the relatively high rock matrix hydraulic conductivity (this phenomenon is a function of the permeability contrast and retention curves of rock and bentonite, see Gens et al. 2002). Initial models of the saturation predicted such a desaturation but these were revised after additional testing and model parametric studies (UPC 1999, Enresa 1998b, 2000). Fig. 3-2 illustrates the tightly coupled processes associated with vapour transport in the buffer.

The basic laws and parameters for hydraulic and thermal processes together with constitutive models of the materials (compacted bentonite and rock) of varying complexity have been used by different modelling groups (Gens et al. 1998, 2009, Alonso et al. 2005, Rutqvist & Tsang 2004, Dupray et al. 2013) both to predict and interpret the overall evolution of the buffer. Model selection and parameters for the bentonite have been based directly on the analysis of extensive laboratory testing (see Fig. 3-3).

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<sup>14</sup> Heat advection is included in the formulation but it turns out to be negligible in this application.

A reference model, the "Operational Base Case" (OBC), was established prior to the start of the two experiments and has been reasonably successful in forward prediction of both instrument measurements and, for the In Situ Test, post-excavation sample characterisation of the buffer around Heater # 1. However, there are discrepancies in the prediction of the speed of saturation in the Mock-up Test that have been addressed by inclusion of either second order processes (thermal osmosis, see Sánchez et al. 2010), refinement of the constitutive laws for the bentonite (double structure models, existence of threshold hydraulic gradients) or by variation of model parameters. These subsequent model developments have included inverse modelling/calibration approaches to existing data together with a prediction of the future response (essentially a history-matching approach) rather than the initial forward modelling method.

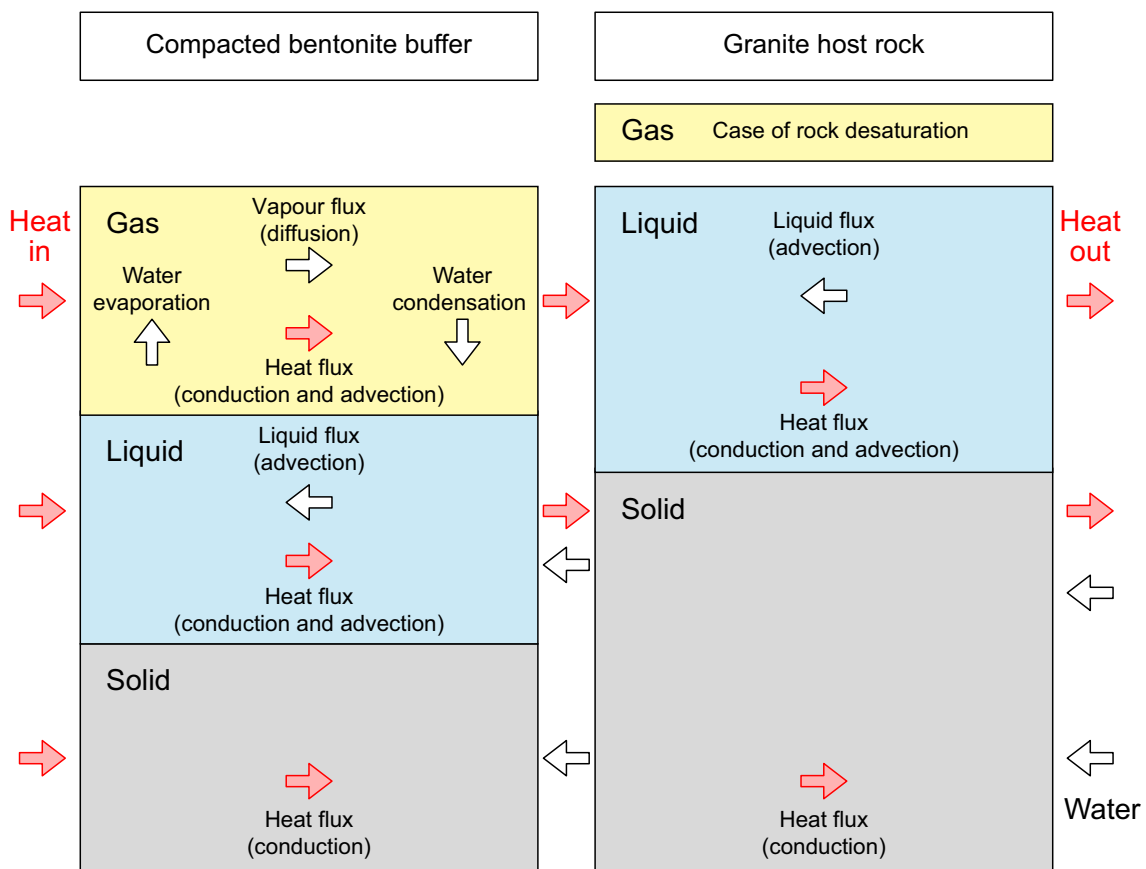


Fig. 3-1: Water, vapour and heat fluxes in buffer and geosphere after Gens (2003).

Refinements to constitutive models of the bentonite have focussed on explaining the slower than expected saturation in the Mock-up and laboratory tests and have included:

- use of a "double structure" model incorporating descriptions of micro- and macro-porosity (Sánchez et al. 2004, 2012b)
- inclusion of a threshold gradient in the flow law (see Sánchez et al. 2007, Enresa 2006c)

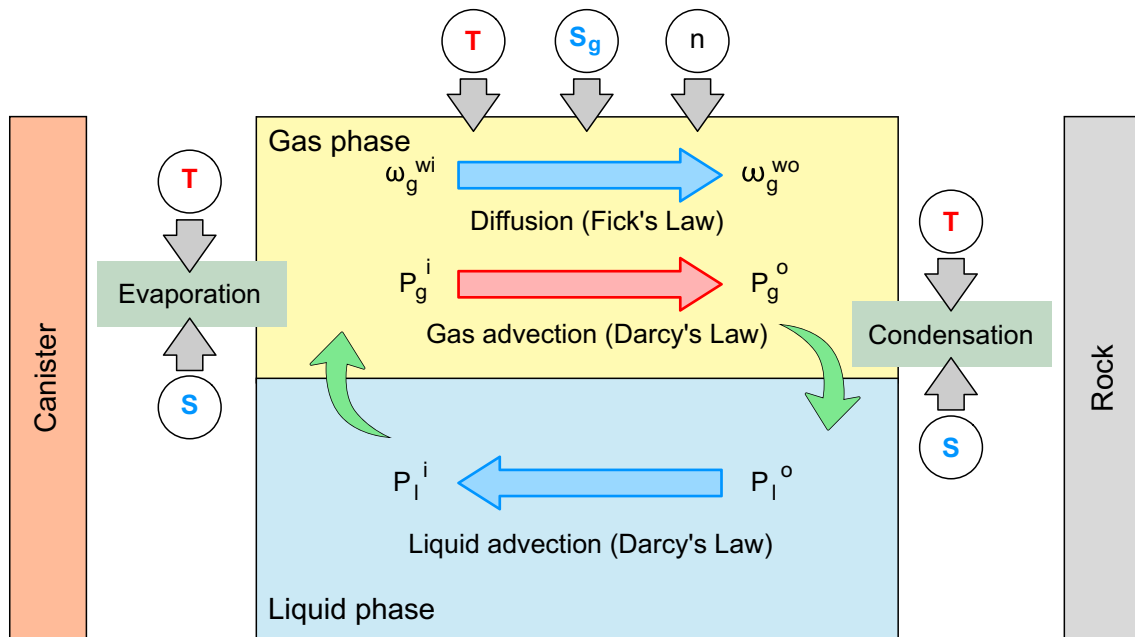


Fig. 3-2: Schematic of coupled processes associated with vapour transport (Gens 2003).

T temperature, S suction,  $S_g$  gas saturation, n porosity,  $\omega_g^w$  mass fraction of water in gas,  $P_g$ ,  $P_l$  gas and liquid pressure. Superscripts i and o refer to the inner (canister) and outer (rock) boundaries of the bentonite.

### 3.1.2 Thermo-hydro-geochemical models

Conceptual THC/THmC models have been based on the THM processes outlined in the previous sections. The fluid and thermal fluxes shown in Fig. 3-1 control the mixing of the bentonite porewater and granite porewater and their reactions with the bentonite minerals. Multiple conceptual geochemical models (CGM) for the bentonite porewater were considered on the basis of the datasets used (obtained from squeezing tests or from aqueous extracts):

CGM-0: Squeezing data (Samper et al. 2001)

CGM-Ciemat: Squeezing and aqueous extraction data (Fernández et al. 1999, 2001)

CGM-1: Aqueous extraction data (Samper et al. 2005a)

CGM-2: Modified version of CGM-1 including squeezing data (Samper et al. 2005a)

The models reflect different balances between the two porewater datasets. The datasets are affected by the artefacts induced by the two methods: squeezing and aqueous extraction.

Consideration of the influence of mechanical processes has focussed on swelling and associated changes in porosity via simplified models (Zheng et al. 2011). Transport mechanisms include: advection, molecular diffusion and mechanical dispersion. The chemical processes considered in the models have developed over time to include: aqueous complexation, acid-base reactions, mineral dissolution/precipitation, cation exchange and surface complexation (Zheng et al. 2011). Additional processes regarding possible  $\text{CO}_2$  degassing have also been suggested.

## 3.2 THM numerical models

### 3.2.1 Modelling using CODE\_BRIGHT

Versions of the Operational Base Case (OBC) models were set up prior to the start of the experiments for both the Mock-up and In Situ Test (see Enresa 1998a, Gens et al. 1998). For the In Situ Test the model is not strictly a "Class A" prediction (Lambe 1973) as the initial operation and model definition overlapped for a few months at the start of the test (Gens et al. 2009) due to uncertainty on the initial power-up schedule and integration of laboratory test results (bentonite permeability and retention curve). However, given the length of the experiment, the OBC model results can reasonably be considered true "blind predictions" of system performance. The models of the two tests differ in respect of the differences in geometry, initial conditions (in particular dry density) and boundary conditions.

Fig. 3-3 illustrates the sub-models and data sources for the OBC (Gens et al. 2009) and Double Structure (DOU) (Sánchez et al. 2012a) bentonite models. The complexity of the model in terms of the number of sub-models and parameters can be clearly seen.

Within the OBC model (Gens et al. 2009), the mechanical behaviour of the bentonite is represented by a modified form of the Barcelona Basic Model (BBM) (Alonso et al. 1990). Within the DOU model (Sánchez et al. 2012a) the bentonite is represented as two overlapping continua (macrostructure and microstructure) as described in Sánchez et al. (2005) in a modified form of the Barcelona Expansive Model (BExM) (Alonso et al. 1999). The application of the DOU model to laboratory tests on the FEBEX bentonite is demonstrated in Lloret et al. (2003).

For the In Situ Test, the OBC model provides good quantitative prediction of temperature, relative humidity, water content and dry density up to removal of Heater # 1 (Gens et al. 2009). Stresses are less well predicted, in part because of greater variability in measurements but more generally indicating a slower development of stress than predicted by the model. Subsequently, higher stresses than predicted by the model are developed at some sensors. These may indicate the effect of initial joint closure (delay in stress development) and contact variability induced by the joints. Conversely, measurements from dismantling show a high degree of uniformity.

Sánchez et al. (2012b) present modelling of the cooling and partial dismantling of the In Situ Test and subsequent evolution using data up to day 3'761, also providing a prediction for a 20-year period using the OBC. The model implements a new CODE\_BRIGHT excavation module. The model predicts near full saturation in zones away from the remaining heater, but continued low saturation in sections close to the heater with strong thermal gradients.

Within FEBEXe, a revised model of the In Situ Test has been developed to take advantage of recent code developments. The model allows more flexible handling of meshes and boundary conditions that simplify simulation of dismantling (Olivella et al. 2012). The model results have been compared with the OBC model up to removal of Heater # 1 and are in good agreement. Simulations of the post-partial dismantling behaviour again show reasonable agreement with temperature measurements. Matches to relative humidity and stress are less good than those to temperature. Sensitivity studies included changes in the relative permeability curve, use of the double structure model, inclusion of thermo-osmotic flow and an increase in bentonite intrinsic permeability (water saturated). A permeability increase of a factor of 2 caused the most obvious improvement in match to the observations.

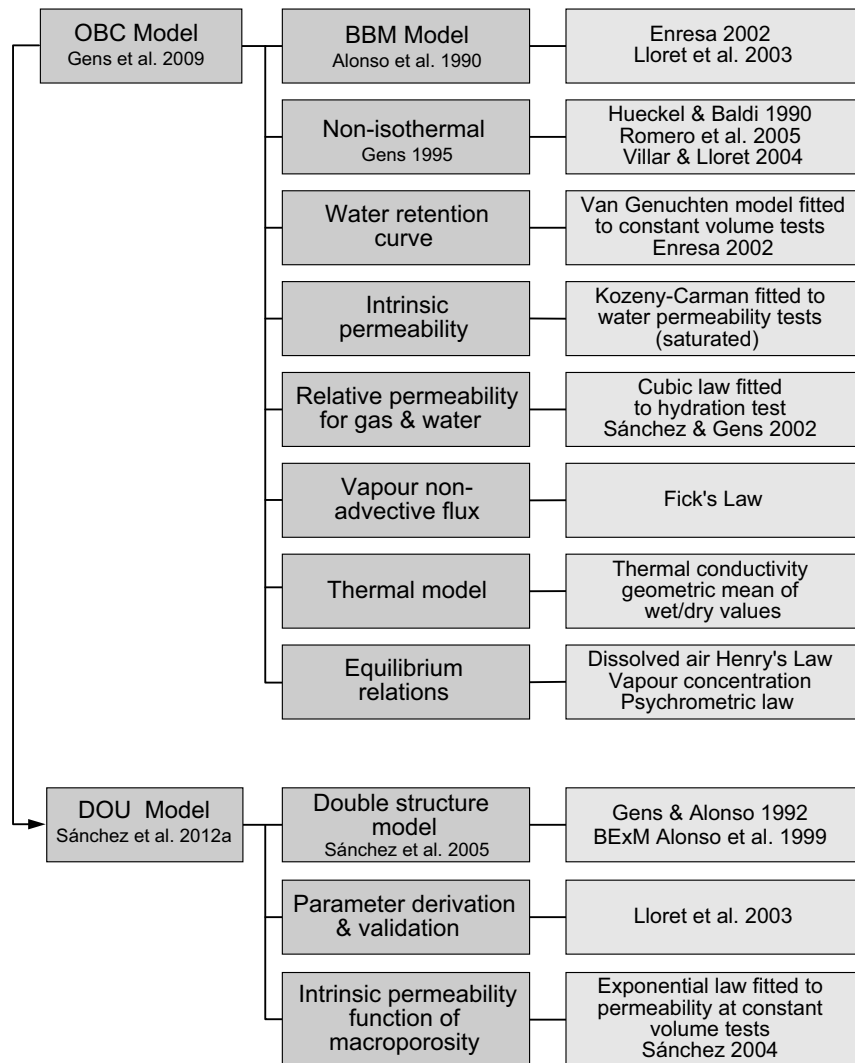


Fig. 3-3: Constitutive models and data sources used in the OBC and DOU models.

In summary, the OBC model and its development (Olivella et al. 2012) have demonstrated a good predictive capability over the fifteen years of operation of the In Situ Test with many of the qualitative patterns being matched by the models and some measurements showing good quantitative matches. Inclusion of additional processes (thermo-osmosis), refining constitutive laws (threshold gradient) or including a double structure model have all been considered but have not noticeably improved the match to the In Situ Test data for the parameter range investigated. A factor 2 increase in permeability (roughly equivalent to a  $0.1 \text{ Mg/m}^3$  reduction in dry density) did however improve the match. Further analyses were performed within the PEBS Project<sup>15</sup>.

A fully coupled THMC version of the CODE\_BRIGHT code and its application to the In Situ Test (prior to partial dismantling) has been presented in Gens et al. (2010) with a simulation covering a period over 100 years to predict long-term THMC conditions.

<sup>15</sup> PEBS (Long-term Performance of Engineered Barrier Systems) was a 7<sup>th</sup> EURATOM project to evaluate the sealing and barrier performance of clay-based EBS over time.

With regard to the Mock-up, Sánchez et al. (2012a) describe modelling to day 3'421. In their evaluation of the OBC, they suggest that:

- Temperature measurements are generally well predicted by the OBC model.
- The overall speed of buffer hydration is overestimated in comparison with the total water intake, resulting in a significant underestimate of the time for full saturation.
- The model achieves a reasonable match of hydraulic, thermal and stress observations close to the heaters up to 900 days, with increasing departure from measurements after this.
- A slight departure from predicted behaviour relatively late in test (from day 2'000?).

Several possible causes of the overall slowing of saturation of the Mock-up were investigated, including:

- uncertainty in parameters (sensitivity) of constitutive laws (Sánchez & Gens 2002)
- evaluation of the effect of "air-tightness" on the saturation – no significant effect was found for two bounding cases: free flow of air in and out of the experiment or a completely airtight experiment

Additional checks were also made to ensure that the measured flow rates were accurate and that the observed slowing of saturation was real (Enresa 2006c, Sánchez et al. 2012a, see also discussion in Appendix B). A comparison of the predictions from the double structure model with oedometric tests on compacted FEBEX bentonite is presented in Lloret et al. (2003). The pre-consolidation stress parameter in the models was adjusted to account for the overall lower density in the Mock-up than in the oedometric tests. Use of the DOU model provides a significant improvement in the match to observation. The DOU model predicts well the overall slowing in saturation as shown in water uptake (hydration locking) and measurements of relative humidity and stress. Other possible influences on the speed of hydration are:

- the existence of an hydraulic gradient threshold for flow (Enresa 2006c, Sánchez et al. 2007)
- variation of hydraulic conductivity with ionic strength of porewater (McNeal & Coleman 1966, Enresa 2002)
- effect of thermal osmosis (Enresa 2006c, Sánchez et al. 2010)

In summary, bentonite saturation under hydraulic and thermal gradients relevant to repository conditions has been studied from the laboratory-scale to full-scale (In Situ Test). However, larger-scale tests have typically not been able to attain high saturation throughout the bentonite. In part, this reflects the expected low permeability of the compacted bentonite but models of the FEBEX In Situ Test, Mock-up Test and 40 cm infiltration tests (I-40, GT-40) suggest that this does not fully account for the length of time required for saturation as observed in the laboratory. Tab. 3-1 presents a comparison of the different hypotheses related to the slower than expected saturation (see also Appendix B for an evaluation of the slowing observed in the Mock-up Test). It can be seen that no single model explains all the observations and that several models can explain at least some of the deviations from the expected performance derived from the standard OBC model.

Tab. 3-1: Models of bentonite saturation for 40 cm infiltration tests (I-40, GT40), Mock-up and In Situ Test.

	Effect on saturation	Tests I40, GT40	Mock-up Test	In Situ Test	Relevance to repository
Timescale		Data to ~ 3.5 years	> 15 years	> 15 years	10 s – 1'000 s of years
OBC model	Standard THM model calibrated to extensive lab testing (Gens et al. 2009)	Unsatisfactory match, especially for GT40 (Sánchez et al. 2007)	Overpredicts rate of saturation (Enresa 2006c)	Reasonable match to relative humidity and temperature. Less good match to stress (Olivella et al. 2012)	Standard model approach implemented in existing programmes
Double structure model	Macro-porosity reduces with hydration, reducing permeability/advective flux (Sánchez et al. 2005)	Evaluation in progress	Improves global and local matches (Sánchez et al. 2012a)	Less good match (Olivella et al. 2012) *	Slows and delays achievement of high water saturation
Threshold gradient	At low hydraulic gradient advective flux is zero with non-linear response below critical gradient	Improves match GT40 but underestimates flow in I40	Improves match (Enresa 2006c)	Not evaluated	Delays saturation while thermal gradient sufficient to balance advective flux and reduce gradient
Thermo-osmotic flow	Thermal gradient creates counter movement of water that may "balance" advective water flux	Improves match close to heater in GT40. No effect for I40	Improves match (Sánchez et al. 2010). High thermal gradient in Mock-up increases influence	Less good match (Olivella et al. 2012)	
Parameter variation	Parameter changes influence advective flux on saturation	Not evaluated	Variants performed could not explain slowing saturation	Improvement from factor 2 permeability increase	Standard model approach implemented in existing programmes

\* Results were reviewed and further analyses performed as part of the PEBS project.

### 3.2.2 Modelling in DECOVALEX

The FEBEX In Situ Test was modelled within the framework of the DECOVALEX III Project (Stephansson et al. 2004, Tsang et al. 2005). The modelling exercise, aimed at predicting in situ behaviour, was organised in three parts (Alonso & Alcoverro 2005, Alonso et al. 2005):

- Part A: Hydro-mechanical modelling of the host rock. Predictions for the total water inflow and pressure changes induced by excavation.
- Part B: Thermo-hydro-mechanical modelling of the bentonite. Predictions for temperature, relative humidity, stresses and displacements at selected points in the bentonite buffer (up to day 1'000).
- Part C: Thermo-hydro-mechanical modelling of the near-field host rock. Predictions for temperature, stresses, water pressures and displacements in the host rock were required.

Ten modelling teams from Europe, North America and Japan were involved in the analysis of the test. Differences among approaches may be found in the constitutive models used, in the simplifications made to the balance equations, and in the geometric symmetries considered. An extensive data set was developed and delivered to the DECOVALEX modelling teams.

The major conclusions from the project (Alonso et al. 2005) were:

- Success in numerical modelling relies mainly on proper hydrogeological characterisation of the rock mass and experimental system, and less on the choice of a particular numerical approach (discrete fractures system or equivalent porous continua).
- Fully coupled hydro-mechanical models need to be applied to simulate/predict the flow and stress/deformation behaviour of fractured rocks, especially when excavation is involved, since the latter presents a significant transient mechanical loading mechanism and change of boundary conditions.
- Predicting the behaviour of the bentonite buffer under combined heating and wetting actions requires a fully coupled THM formulation, which incorporates all the necessary physical processes present in the bentonite<sup>16</sup>.
- Particularly relevant for predicting the early stages of heating was the inclusion of phase changes of water and the vapour transport in the bentonite.
- The hydration of the bentonite buffer was essentially independent of the heterogeneous nature of the hydraulic conductivity distribution in the surrounding rock, when the rock matrix permeability is much higher than the saturated bentonite permeability.
- Heating of the rock had a significant effect on rock stresses in the vicinity of the FEBEX tunnel, but much less on water pressures – a result, perhaps, of the relatively high rock permeability.

While the quality of match to observations varied between the three parts, performance measures and modelling groups, Alonso et al. (2005) note that the coupled models of SKB and SKI "achieved a good overall representation of the buffer response against the combined action of heating and external wetting" in Part B. Further, the SKI model (Rutqvist & Tsang 2004) achieved "a consistent prediction of all the measured variables in the rock" in Part C.

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<sup>16</sup> Inverse modelling of the In Situ Test using only thermo-hydro (TH) coupling is currently under way within the PEBS Project and shows the potential for achieving reasonable matches to observations using a restricted set of processes coupled with an inverse approach to parameter estimation.

More detailed discussions of the different groups' FEBEX modelling within DECOVALEX can be found in Alonso et al. (2005). Papers by individual modelling groups are included in Stephansson et al. (2004) and a special volume (42, issues 5 – 6) of the International Journal of Rock Mechanics and Mining Sciences.

Tab. 3-2: Modelling teams, codes and key couplings for simulation of the buffer evolution (Part B) of DECOVALEX III FEBEX Task.

Team	Couplings	Numerical code	Deformation	Dimension	Liquid ↔ gas <sup>17</sup>	Vapour flux	Permeability Kw(Sr) <sup>18</sup>	Thermal cond. $\lambda_1$ (Sr) <sup>19</sup>	Suction → deform. ev(Sr) <sup>20</sup>
Andra	Information not available in Alonso & Alcoverro (2005)								
BGR	TH⇒HM	RF/RM		2		X	X		X
CNSC	THM	FRACON	X	3	X	X	X		X
USDOE	TH⇒TM	THOUGH2/JAS3D	X	3	X	X	X		
IRSN	THM	CGEF/HYDREF/VIP LEF	X	1			X		
JNC	TH	THAMES3D		3		X	X		
SKB	THM	ABAQUS	X	2	X	X	X		
SKI	THM	ROCMAS	X	3	X	X	X		
STUK	TH	ELMER		1	X	X	X		

Andra – Agence Nationale pour la Gestion des Déchets Radioactifs, France; BGR – Federal Institute for Geosciences and Natural Resources, Germany; CNSC – Canadian Nuclear Safety Commission; USDOE – U.S. Department of Energy; IRSN – Institute for Radiological Protection and Nuclear Safety, France; JNC – Japan Nuclear Cycle Development Institute; SKB – Swedish Nuclear Fuel and Waste Management Company, Sweden; SKI – Swedish Nuclear Power Inspectorate; STUK – Radiation and Nuclear Safety Authority, Finland.

Andersson (2005) evaluated the relevance to performance assessment of THM coupled processes within Task 4 of DECOVALEX III. He stated that while the "bentonite buffer and its interaction with the near-field rock is an essential component of most deep geological repository concepts [...] for repository performance, the outstanding issue is to assess the barrier performance over long times. Details in the re-saturation phase are not necessarily important unless they would imply long term remaining effects." As the FEBEX modelling task focused on short-term response, Anderson (2005) concluded that the long-term issues remain to be addressed.

<sup>17</sup> Phase change between liquid water and water vapour.

<sup>18</sup> Saturation-dependent water permeability.

<sup>19</sup> Saturation-dependent thermal conductivity.

<sup>20</sup> Suction-induced deformations.

### 3.2.3 Modelling using LAGAMINE

Within FEBEX an alternative THM model using the ACMEG-TS elasto-thermoplastic constitutive model (Laloui & Francois 2009) with the LAGAMINE code has been developed by EPFL (Francois & Laloui 2009, Dupray et al. 2013). In an initial phase of the study, models of the first operational phase (up to switch-off of Heater # 1) were presented in Dupray et al. (2013). The model has been applied to the In Situ Test only.

The parameters of the thermoplastic constitutive model were derived from back analysis of oedometer tests under controlled suction and temperature conditions while those for hydraulic and thermal diffusion were taken from literature. The bentonite parameters were based on the compacted block density  $1.70 \text{ Mg/m}^3$  rather than the volume-averaged density  $1.60 \text{ Mg/m}^3$  – including gaps between blocks – but partially compensated for this by reducing the thermal output of the heaters by 15 % to account for heat transfer along the air gaps. In the short term this assumption probably results in an overestimate of swelling pressure, while the long-term effects, when the gaps have largely closed (as seen during dismantling), are unclear. The models achieve a quantitative match to the observed temperature and more qualitative matches to measured relative humidity, stress and displacement. The models were not compared with the results from dismantling.

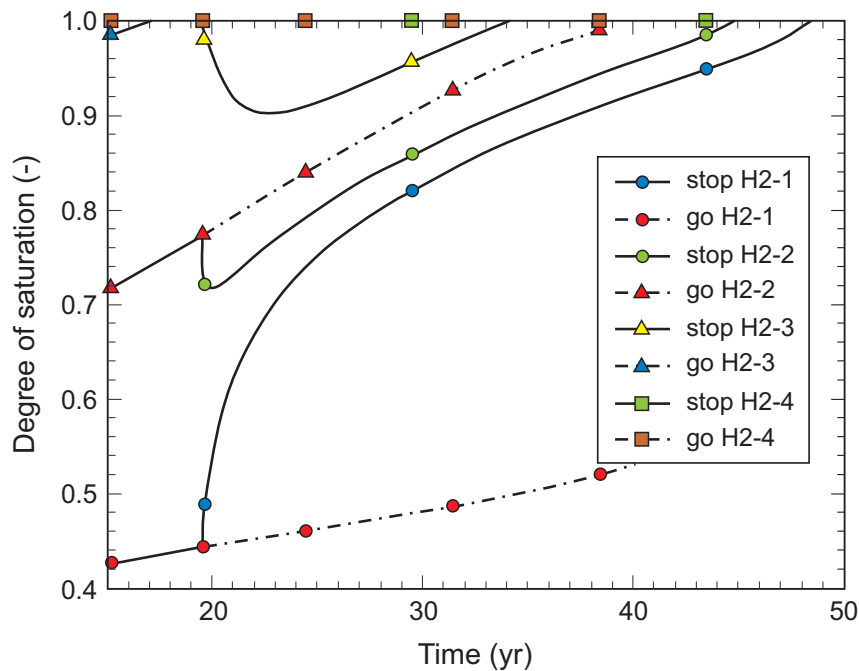


Fig. 3-4: Evolution of saturation from the stopping date (18 years) in model Section H2 (corresponding to sensor Section F2 at the mid-line of Heater # 2) from recent LAGAMINE simulations for "stop" and "go" cases.

Point H2-1 is located next to the heater, H2-4 next to the rock. H2-2 & H2-3 are intermediate points.

In a second phase, the simulations were extended to cover switch-off and excavation of Heater # 1 and the second operational phase (Dupray 2013). The models achieved a good overall match to temperature, although the effect of switching off Heater # 1 was overestimated close to the heater. Qualitative agreement with the measured relative humidity was achieved,

but only limited match to the stress data was possible – although this may be due to issues with the measurement of stresses in the buffer. Models were run for a simulation period of 31 years. Within the models, full saturation was not achieved close to Heater # 2 even in this time, and saturation time was estimated to be 30 to 40 years.

Two variant simulations have been performed, one – labelled "stop" – where Heater # 2 is switched off in February 2015 (after 18 years of saturation), and the other – labelled "go" – where heating continues. When heating is stopped, there is a relatively fast redistribution of moisture from the outer buffer towards the heater, which is followed by slower ongoing saturation. Full saturation at the heater is achieved after 48 years in the "stop" simulation while saturation is still ongoing in the "go" case.

### 3.2.4 Summary

The ACMEG-TS and OBC models incorporate similar processes with somewhat different constitutive models, both with material parameters calibrated to laboratory-scale tests. Overall, both models can claim quantitative reproduction of the observed temperature responses, a reasonable match to relative humidity and more qualitative matches to other parameters (as can some of the DECOVALEX models discussed in the previous section). Sensor effects (local conditions, block contacts, gaps, sensitivity) influence other measurements more than temperature and partly explain the lower quality of match. In addition to the sensor data, there was very good agreement between the OBC model predictions and the dismantling data after five years of heating. Therefore, sample data from the final dismantling and sensor data from the Mock-up may be more useful datasets to evaluate the two models than the In Situ Test sensor data.

Early design models of the In Situ Test (Gens et al. 1998) suggested relatively quick saturation (~ 4 – 5 years) apart from cases where desaturation of the rock occurred (creating a capillary barrier to flow from the geosphere). These models assumed an intrinsic reference hydraulic conductivity for the bentonite of approximately  $2 \times 10^{-13}$  m/s. Subsequent models (OBC) assumed a hydraulic conductivity of  $\sim 2 \times 10^{-14}$  m/s resulting in significantly longer saturation times. Tab. 3-3 lists the recent predictions from selected models. It can be seen that full saturation around Heater # 2 would not have been achieved in any reasonable experimental timescale.

Tab. 3-3: Predicted saturation times for selected models of the In Situ Test.

Model case	Saturation prediction
UPC: OBC	Full saturation in cold sections, but not achieved at Heater # 2 after 20 years (Sánchez et al. 2012b, Olivella et al. 2012)
EPFL: ACMEG-TS go	Full saturation at Heater # 2 not achieved after 50 years (Dupray 2013)
EPFL: ACMEG-TS stop	Full saturation at Heater # 2 after 48 years (Dupray 2013)

### 3.3 THC/THmC numerical models

One of the objectives of the FEBEX project was the study, identification and modelling of the possible geochemical alterations in the engineered barrier due to the combined effect of high temperatures and water flow. A detailed and extensive laboratory programme was carried out in order to provide thermo-hydro-geochemical (THG or THC) parameters and identify the processes triggered by temperature and water flow.

This section presents a brief overview of THC/THmC modelling of laboratory experiments, and Mock-up and In Situ Tests. These THC/THmC models rely on flow, thermal, transport and geochemical conceptual models discussed previously. Multicomponent solute transport mechanisms include advection, molecular diffusion, and mechanical dispersion. Chemical reactions considered in the models include: aqueous complexation, acid-base, calcite, quartz/chalcedony and gypsum/anhydrite dissolution/precipitation,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  cation exchange, and proton surface complexation.

The THC numerical codes used include: CORE: CORE<sup>2D</sup> V4 (Samper et al. 2003, 2011), FADES-CORE (Juncosa 2001), INVERSE-CORE<sup>2D</sup> (Dai & Samper 2004) and INVERSE-FADES-CORE (Zheng & Samper 2004 and 2005). A more detailed summary of the UDC modelling is presented in Appendix C.

#### 3.3.1 Models of laboratory tests

Many different types of laboratory experiments were performed to support the Mock-up and In Situ Tests. The modelling and interpretation work was performed by UDC in close cooperation with CIEMAT.

#### **Squeezing and aqueous extract tests (AET) at different durations and different S/L (Solid/Liquid) ratios**

Initial bentonite porewater composition was obtained by inverse hydrogeochemical modelling using the reactive transport code CORE<sup>2D</sup> (Samper et al. 2003). The performance of the conceptual models CGM-1 and 2 (see Section 3.1.2) were evaluated. It was found that CGM-1 could not fit the squeezing data while CGM-2 was able to simultaneously fit both aqueous extract data and squeezing data, although there were clear deviations for sulphate.

#### **Inverse hydrochemical modelling of AET of samples from the In Situ Test**

Zheng et al. (2008) present an inverse hydrochemical model to estimate porewater chemical composition from measured water content, aqueous extract, and mineralogical data taken from samples at different radial distance on dismantling Sections 19 and 29, located at the edges of Heater # 1. The inverse method using INVERSE-CORE<sup>2D</sup> (Dai & Samper 2004) and accounted for a wide range of chemical processes including: acid-base, redox, aqueous complexation, mineral dissolution/precipitation, gas dissolution/ex-solution, cation exchange and surface complexation reactions, all of which were assumed to take place at local equilibrium. The inverse model reproduced most of the measured aqueous data except bicarbonate. The main uncertainties were related to kinetic calcite dissolution and variations in  $\text{CO}_2(\text{g})$  pressure.

### **THC modelling of the permeation test**

Samper et al. (2005b) and Enresa (2006a, 2006d) present THC modelling of a long-term permeation test on a 2.5 cm long sample of saturated FEBEX bentonite (Fernández et al. 2002). In the test, the saturated bentonite sample was flushed with granitic water over a period of 4 years. Samper et al. (2008b) presented an updated inverse single- and dual-continuum multicomponent reactive transport model. The model accounted for solute advection and diffusion and geochemical reactions such as aqueous complexation, acid-base, cation exchange, protonation/deprotonation by surface complexation and dissolution/precipitation of calcite, chalcedony and gypsum. The initial composition of bentonite porewater used was derived from a squeezing experiment (CGM-0, Samper et al. 2005a). It was found that breakthrough curves of reactive species were more sensitive to initial porewater concentration than to the effective diffusion coefficient and optimum estimates of the initial FEBEX bentonite porewater chemistry were obtained by inverse modelling of multicomponent reactive transport. The single-continuum model (SCM) reproduced the measured trend for most chemical species but failed to match the long tails of most breakthrough curves, while dual-continuum models (DCM) were also able to match the tails.

### **THC/THmC modelling of the CT23 test**

The CT23 test was one of a series investigating water flow and reactive solute transport in compacted bentonite during simultaneous heating and hydration (Huertas et al. 2000). Zheng et al. (2010), following previous THC modelling (Samper et al. 2005b, Enresa 2006a, 2006d), present a non-isothermal multiphase flow and multicomponent reactive solute transport model in a deformable medium (THmC model). The THM model was calibrated with transient temperature, water content and porosity data measured at the end of the experiment. The reactive transport model was calibrated with porewater chemical data derived from aqueous extract data. Computed concentrations agreed well with inferred aqueous extract data at all sections except near the hydration boundary, where cation data are affected by sampling artefacts.

#### **3.3.2 Models of the Mock-up Test**

THC and THmC models of the Mock-up Test were developed to predict the transport patterns of added artificial tracers (iodide) and predict the THC/THmC performance of the engineered barrier of the Mock-up Test (Enresa 2000, Samper et al. 2005b, Enresa 2006a, 2006d).

Zheng & Samper (2008) present the most recent THmC model of the FEBEX Mock-up Test. This 1D axisymmetric coupled THmC model accounted for thermal and chemical osmosis and bentonite swelling with a state-surface approach and reproduced the measured temperature and cumulative water inflow data. The model matched the relative humidity in the outer part of the buffer but underestimated relative humidity near the heater. Dilution due to hydration and evaporation near the heater were the main processes controlling the concentration of conservative species, while proton surface complexation, mineral dissolution/precipitation and cation exchange also significantly affected reactive species.

#### **3.3.3 Models of the In Situ Test**

Samper et al. (2008a) present a THC model of the In Situ Test up to dismantling, utilising a common thermo-hydraulic model and three different geochemical conceptual models for the bentonite porewater. The model achieves a good match to temperature in the buffer and the general trend of water content. However, the overall shape of the water content is not matched

as the model assumes a constant temperature boundary condition and does not account for swelling and hence the observed gradient in dry density (Villar et al. 2005). The models reproduce the general trend of  $\text{Cl}^-$  and cations (effectively acting as a conservative tracer) but systematically underestimated  $\text{SO}_4^{2-}$  concentrations. The pattern of  $\text{HCO}_3^-$  concentration data was not fitted well by any of the models which may relate to  $\text{CO}_2$  degassing which the models did not account for.

Zheng et al. (2011) present the most recent THMC modelling of the FEBEX In Situ Test. The model is a development of the previous work by Samper et al. (2008a), who reported significant discrepancies between calculated and measured concentrations for most chemical species. The revised model Zheng et al. (2011) includes thermal osmosis and bentonite swelling to address the problems identified by Samper et al. (2008a) and builds on the model developed for the Mock-up (Zheng & Samper 2008). Sensitivity analyses are used to understand the influence of different assumptions. The model demonstrates the influence of intrinsic permeability, bentonite swelling and thermal osmotic permeability on the porewater chemistry. Inclusion of a state-surface bentonite swelling model together with thermal osmosis allows a reasonable match to the  $\text{Cl}^-$  and cations which largely follow the  $\text{Cl}^-$  trend ( $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ). The models show very little influence of chemical osmosis. Zheng et al. (2011) also demonstrate the importance of calcite dissolution, cation exchange reactions and gypsum/anhydrite dissolution/precipitation on the geochemical evolution of the buffer.

Model results deviate from measurements at the interfaces. Close to the heater and rock, it is suggested that this may be due to several processes such as  $\text{CO}_2$  degassing, bentonite volume changes, vapour transport to the rock or a combination of these.  $\text{HCO}_3^-$  and pH data cannot be explained by the model. Zheng et al. (2011) suggest that this may be due to  $\text{CO}_2$  degassing and transport within the buffer. Significant uncertainties associated with the models therefore remain and include:

- magnitude of thermal osmotic permeability
- accessibility of water within the different porosities in the bentonite
- quantity of gypsum in the bentonite available for dissolution and dissolution mechanism
- initial bentonite porewater composition (see Fernández et al. 2004, Fernández & Rivas 2005, Zheng et al. 2008)
- assumption of a closed (airtight) system

### 3.3.4 Summary

During FEBEX THC/THmC models have been developed and used to:

- interpret laboratory tests for parameter estimation
- interpret laboratory tests to identify relevant geochemical processes
- predict the transport patterns of artificial tracers in both the Mock-up and In Situ Tests
- predict the THC performance of the engineered barrier for the Mock-up and In Situ Tests
- test TCH predictions with dismantling data from around Heater # 1 at the In Situ Test

The ability of the models to reproduce most of the observed THC patterns in these tests gives confidence in their capabilities as diagnostic tools.

## 4 Evaluation

### 4.1 Buffer performance

Within previous performance assessments, the results from FEBEX have been used to support the arguments concerning the bentonite buffer regarding:

- homogenisation of bentonite blocks (Andra 2005)
- thermal behaviour of the buffer including saturation dependent thermal conductivity (Andra 2005, SKB 2006)
- behaviour under disposal conditions (SKB 2011)

The functions of the bentonite buffer in a KBS-3 type repository are illustrated in Fig. 4-1. The functions of the buffer and associated safety functions are presented here in the context of a KBS-3V type repository as a comprehensive safety assessment for such a repository has recently been completed by SKB (2011).

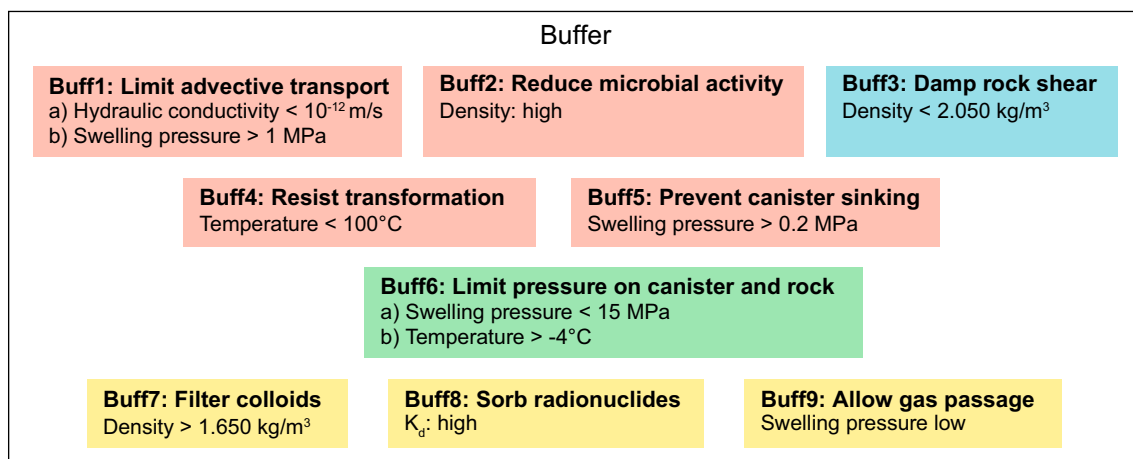


Fig. 4-1: SKB's buffer safety functions for a KBS-3V repository (from SKB 2011).

In a clay host rock, Nagra (2002) specify that the bentonite buffer acts "as a well-defined interface between the canisters and the host rock, with similar properties as the host rock, that ensures that the effects of the presence of the emplacement tunnels and the heat-producing waste on the host rock are minimal, and that provides a strong barrier to radionuclide transport and a suitable environment for the canisters and the waste forms".

Issues that might affect buffer performance in the long term are:

- reliability and homogenisation of buffer properties
- erosion and piping of the bentonite (at emplacement and as a result of flushing of low-salinity water through the repository)
- geochemical processes within the buffer
- bacterial processes within the buffer

### Reliability and homogenisation of buffer properties

A key outcome from FEBEX has been the confirmation that buffer properties derived from small-scale laboratory tests can be successfully applied or upscaled to describe larger-scale tests. Further, it has been shown that models derived at small scale can be used to predict large-scale tests. Evidence for ongoing homogenisation of the buffer can be seen in:

- strongly symmetric (about the central vertical plane) responses in the Mock-up indicating little evidence of any preferential flow (although note the pre-flooding of the Mock-up)
- observed sealing of construction gaps in the buffer during excavation of Heater # 1 in the In Situ Test (see Fig. 4-2)
- distribution of measured dry density during excavation of Heater # 1
- success of homogeneous models of buffer evolution

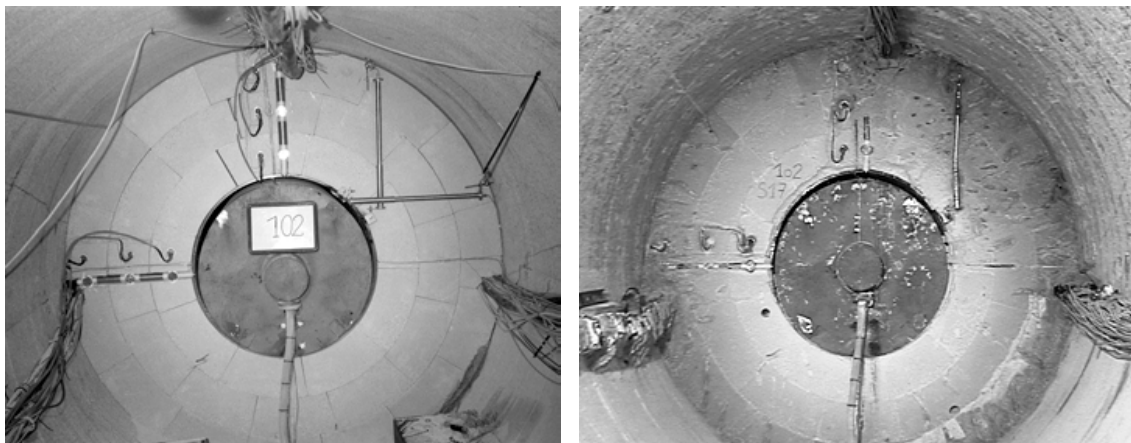


Fig. 4-2: In Situ Test buffer at front of Heater # 1 (Slice 102) during construction (left) and after 5 years of heating (from Svemar & Huertas 2004).

Note closure of construction gaps in and around the buffer.

Again, further evidence will come from the planned dismantling representing a significantly longer (18 years) saturation period.

### Erosion and piping of the bentonite

Inflow to the FEBEX drift is low and so significant erosion or piping of the bentonite would not be expected. Svemar & Huertas (2004) report no problems due to inflows during construction. Sampling from boreholes drilled parallel to the FEBEX drift (Missana et al. 2009) identified bentonite colloids but suggested that, despite experimental difficulties, at ~ 30 cm from the bentonite, the quantity of bentonite colloids cannot be higher than 1 ppm. The bentonite colloids are likely to have been generated by erosive processes (chemical, see Section 2.1.3, or mechanical) at the interface between the bentonite and groundwater. Further observations from the planned dismantling are likely to confirm the lack of any significant fraction of the bentonite due to erosion or piping<sup>21</sup>.

<sup>21</sup> Inflows were noted in the end of the drift around Fr-5 fracture zone by Guimerà et al. (1996).

### **Geochemical processes within the buffer**

Analysis of sample data from 5 years saturation (Enresa 2006b), together with information from up to 8 years of saturation in the 60 cm cells (Fernández & Villar 2010), shows a relatively consistent pattern of porewater evolution in the bentonite. Dilution and evaporation due to hydration from the rock and heating are controlling the transport of conservative species. Dissolution/precipitation and exchange reactions influenced the distribution of non-conservative species.

There has been significant development of THMC models during FEBEX, facilitated by the well-defined THM framework and the data from dismantling. However, fundamental questions regarding conceptual models for the behaviour of the bentonite and associated transport mechanisms (see Birgersson & Karnland 2009) remain open and the applicability of different concepts requires further investigation.

### **Bacterial processes within the buffer**

Very limited characterisation of microbial populations was performed during sampling of the bentonite. Microbially influenced corrosion associated with sulphate-reducing bacteria was identified in one section around Heater # 1, where the sensor configuration may have favoured humidity transport.

Additional data from sections around Heater # 2 after 18 years of saturation and heating would be valuable in evaluating the distribution of microbes and the importance of the instrument channels. The relatively uniform distribution of dry density observed around Heater # 1, with an average dry density of  $1.57 \text{ Mg/m}^3$ , suggests that populations should be low (Stroes-Gascoyne et al. 2011).

Further consideration of the existence of aerobic/anaerobic conditions within the buffer would also be of value for interpretation of both microbial and corrosion processes.

### **Time for saturation of the buffer**

In a repository system, saturation of the buffer will be dependent on the flow from the rock around the tunnel or deposition holes and in relatively "dry" conditions (low matrix permeability) may take from tens of years to several thousand years (SKB 2011). In a clay host rock saturation times may be  $\sim 100$  years (see Senger & Ewing 2008). Typically the safety functions of the buffer assume a fully water saturated state: the buffer needs to be saturated to perform properly. It is, however, believed that no mass transfer can occur between the canister and rock in the unsaturated state and hence no performance is needed prior to saturation (SKB 2011). Nonetheless, it is important to understand the saturation process and any reduction in the uncertainty associated with the timescale for saturation would facilitate arguments concerning the initial buffer state.

Gens et al. (2004) state "a good reproduction of the basic phenomena that affect the THM behaviour of the barrier, including the main interactions, has been achieved" on the basis of experience from FEBEX and the Prototype Repository Project. However, uncertainties remain regarding the observed rate of hydration and specifics of the processes at late time (low gradients) where several hypotheses have been considered regarding the observed rate of hydration:

- presence of a threshold gradient in the formulation of the Darcy equation
- progressive decrease of intrinsic permeability of the buffer due to changes in microstructure
- action of thermal osmosis to counteract flow towards the heater

The evidence from the Mock-up Test clearly indicates a slowing in saturation resulting in stabilisation of the system state. Although any or a combination of these phenomena could explain the observed behaviour, they lead to different long-term predictions, in particular the existence of a threshold gradient might prevent full saturation of the buffer close to the heater/waste (Alonso E. E. in SKI 2003). It is not clear how long it would be necessary to observe the systems under the current boundary conditions to discriminate between hypotheses, or whether a change in boundary conditions would allow model discrimination. The time-scales and uncertainties associated with large-scale experiments may limit the ability to further discriminate between mechanisms at low-gradients when forces are closely balanced. An alternative approach would be to perform additional small-scale testing under well-controlled boundary conditions (e.g. tests under constant temperature and a range of gradients) aimed at discriminating between the mechanisms. The understanding from these tests can then be compared with the experience from the large-scale tests.

Slower than expected saturation of EBS components has been observed in some other long-term experiments (see Villlar et al. 2012) including the Gas Migration Test (GMT, Shimura et al. 2008), Isothermal Test (ITT, Dixon et al. 2002<sup>22</sup>). A double structure model (Thomas et al. 2003, 2009) has been used to explain the observed infiltration in the ITT. Apart from the hypotheses considered for the Mock-up Test, other possible reasons for slower than anticipated saturation include:

- higher than expected compacted buffer density – hence lower permeability (e.g. GMT)
- inhomogeneities in buffer density – flow may be controlled by the lowest permeability zones if they are sufficiently continuous
- blocking of flow in the geosphere by bentonite extrusion (see Dixon et al. 2002)
- desaturation of the rock (Gens et al. 1998)

Only the first two are potentially relevant to the Mock-up Test.

## 4.2 Geosphere behaviour

The geosphere response to buffer emplacement and saturation has been largely as expected. Temperatures rose during the first operational period and a radial thermal gradient away from the drift was established. Temperatures dropped after switching off Heater # 1 (net drop in power output) and established a new near-steady state with a slight ongoing upward trend (probably related to the increase in power for Heater # 2). The slight upward temperature trend observed in boreholes suggests that the thermal front is still expanding.

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<sup>22</sup> Dixon et al. (2002) also discuss the faster than expected water uptake for the Buffer Container Experiment.

The wide range of hydraulic diffusivity in the rock resulted in differences in the speed of pore pressure response to sealing of the open drift and to dismantling, but pressures have typically been stable after the first years of the second operational phase. Total pressure (stress) has responded to the development of buffer swelling pressure showing a general radial dependence as would be expected. Models have been able to match the observations reasonably well given the uncertainty in some parameters (e.g. bulk thermal conductivity) and the expected local heterogeneity.

Investigations from FUNMIG<sup>23</sup> (Buckau et al. 2007) found that the flow system had not changed after 12 years with respect to the measurements carried out in the FEBEX project (Missana 2007). Hydraulic gradients are towards the empty part of the gallery. They also identified the influence of near-field water chemistry with an increase in Na and Cl concentration in transmissive borehole sections where the Na/Cl ratio was very close to that of the bentonite porewater. Iodine tracer (included on filter papers in the buffer) was detected in the same sections although rhenium was not (probably influenced by redox conditions). These observations have been compared with predictions for a simple diffusive model of transport in the geosphere (Buil et al. 2010).

In general, the buffer is largely unaffected by geosphere events. A major perturbation in groundwater head distribution occurred in mid September 2006 (~ day 3'520) when packer systems were removed from BOUS 85.001 and BOUS 85.002. Heads were disturbed in almost all surrounding boreholes and took more than 8 months to fully recover, but there is no significant impact on sensor responses in the EBS<sup>24</sup>.

The hydrogeology of the region around the drift has provided a stable environment able to provide sufficient water to the buffer to allow ongoing saturation controlled by the bentonite's ability to take up water. There is no evidence for any significant piping or erosion of the bentonite (this is consistent with the low measured drift inflow). In the small number of locations close to the drift where it has been possible to take samples, bentonite colloid release has been detected but concentrations are below ppm level and transport of bentonite porewater appears to be diffusive (Buil et al. 2010). These samples were taken from relatively low transmissivity fractures ( $10^{-12} - 10^{-9} \text{ m}^2/\text{s}$ ).

Regarding the possible Excavation Damage Zone (EDZ) around the drift, Bazargan Sabet et al. (2003) comment that "All the experimental results show that the granite matrix has not been damaged neither by the excavation nor by the THM loading undergone by the rock mass. Except a zone of about 3 mm depth put to the fore by the SEM/EDX (Scanning Electron Microscopy coupled with Energy Dispersive X-ray Spectroscopy) analyses, the granite seems to preserve its mechanical and hydraulic properties. The evidence of a potential EDZ concerns only the lamprophyre and the interface between lamprophyre and granite." This experience is consistent with other studies of the EDZ around TBM excavations (e.g. Autio et al. 1998), however it should be noted that EDZ occurrence is highly dependent on the excavation method, local stress and host rock conditions, so this conclusion cannot necessarily be applied elsewhere.

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<sup>23</sup> FUNMIG: Fundamental Processes of Radionuclide Migration. An integrated project within EURATOM 6<sup>th</sup> EC Framework Programme.

<sup>24</sup> There is a possible small reaction in total pressure cell 70AIT-PSB2-01 at the end of the drift.

### 4.3 Performance of the FEBEX disposal system

Alonso (2005) notes that while the AGP Granito design remained practically unchanged for many years, lessons learned from Enresa's research programme, especially the FEBEX experiment, were sufficient to warrant a review of the conceptual design. Alonso (2005) states that preliminary conclusions included:

- Reduction of buffer thickness. Previous designs had placed a penalty on the thermal design and performance assessment sensitivity calculations showed that a reduction in thickness had no significant impact on performance.
- Deposition drift diameter can be reduced to 2.0 m taking into account accessibility for construction and operation.
- Elimination of the steel sleeve or liner to facilitate canister deposition.
- Increase in size and water content together with a reduction in dry density of the bentonite blocks.
- New formulation of the thermal constraint for the buffer to avoid an unduly conservative design.
- Development of a methodology for the thermal design.

The FEBEX experiment therefore provided not only demonstration of the feasibility of construction of EBS for horizontal emplacement in drifts, but also provided highly useful information regarding the refinement of designs and procedures.

### 4.4 Performance of instrumentation

Sensors and data acquisition systems have typically functioned well beyond the expected lifetime of the experiments. In the Mock-up Test, 85 % of sensors are still operational after 15 years of operation. Relative humidity sensors show the highest "failure rate" (approx 45 %), although this largely relates to saturation of the sensor, while only about 8 % of temperature sensors are no longer operational. The response to the overheating event, where buffer temperatures reached approximately 200 °C, further demonstrates the robustness of both the instrumentation and the experimental setup in that "no important consequences or irreversible perturbations of the processes or sensors" was evident (Cañamón et al. 2004).

In the In Situ Test, 72 % of sensors were still operational after 15 years. Of the non-operational sensors, 30 % relate to saturation of humidity sensors, while other failures occurred either at installation (4 %), dismantling of Heater # 1 and resealing, or progressively during the experiment. Ongoing failure of some total pressure cells together with the lower initial density of relative humidity and total pressure cells mean that the spatial distribution of these two parameters is less well determined in the In Situ Test than in the Mock-up.

Results from post-excavation characterisation and recalibration further support the quality of the initial design and implementation of the In Situ Test. Sensor recalibration has in some cases provided an improvement in data quality and has been retrospectively applied to data.

## 4.5 Modelling and interpretation

THM modelling has played a significant role in the FEBEX programme from the initial design studies through the experimental period. The major processes controlling the behaviour of buffer/geosphere evolution were identified prior to the start of the experiment and have remained central to almost all successful model simulations (see DECOVALEX III conclusions in Alonso et al. 2005, Tsang et al. 2005).

The OBC model developed by UPC at the start of the test has provided a reference prediction for both the In Situ Test and Mock-up Test. The success of the model in predicting the initial development and continued evolution of the two tests relies on the identification of the most significant processes, detailed laboratory characterisation of the buffer, the limited influence of buffer heterogeneity (e.g. construction joints), and for the In Situ Test, the relative unimportance of the geosphere. Alternative constitutive models based on the same laboratory dataset have also been successful in reproducing much of the observed sensor responses.

The CODE\_BRIGHT models from UPC, LAGAMINE models from EPFL and some of the models from DECOVALEX have been able to provide acceptable predictions or simulations<sup>25</sup>. For the most part, these models represent the same basic physical processes although using somewhat different constitutive laws and associated parameters. Within this study, it has not been possible to forensically evaluate the performance of the different models to determine the key factors in achieving matches to the observations. However, Alonso et al. (2005) give some comments on key requirements for modelling of the In Situ Test.

In the Mock-up, there is evidence for a significant slowing of saturation that is not easily explained by the parameter uncertainty associated with the models and has been the focus of attempts to update the models by considering additional processes or refining process descriptions. The refined models can better reproduce the observed slowing and are based either on refined descriptions of the bentonite structure or previously identified uncertainties in bentonite behaviour. There appears to be no unique model that explains all results and it is possible that some combination of the refined structural or process descriptions is responsible. It is also possible that other processes (see discussion in Appendix B) have resulted in reduced inflow and consequent slowing of saturation in the Mock-up. The evidence for a similar slowing in the In Situ Test is less clear.

Overall, while THM models have been further refined during FEBEX and there are still uncertainties associated with some couplings and process descriptions, the generally good agreement between models and observations gives increased confidence in the robustness of the models.

Coupled THC/THmC models are necessarily not yet at the same level of robustness as the THM models. Different conceptual models of bentonite porosity, porewater and transport mechanisms are still under discussion. Furthermore, it has not yet been possible to include all the processes thought relevant to porewater chemistry and mineralogy evolution within the buffer.

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<sup>25</sup> Some modelling studies have necessarily been performed largely after the data were acquired and hence cannot be considered as predictions.

#### 4.6 Consideration of the FEBEX objectives

A key objective of the FEBEX experiment, the demonstration of the practicality of the concept, was achieved within the first few years. McKinley & Zuidema (1999) describe FEBEX as a good example of an experiment focusing on "Demonstration and Validation" in that the "practicality of implementing a disposal concept for spent fuel in a crystalline host rock was demonstrated on a 1:1 scale". In addition, they note that the experiment provided:

- monitoring data to test coupled models of THM and THC processes
- information on sensor longevity and system decommissioning (relevant to monitoring and retrievability)
- valuable input for design optimisation leading to 2<sup>nd</sup> generation concepts providing equivalent or better levels of safety that are more practical and less expensive

A further part of the demonstration came with the dismantling of Heater # 1 and the confirmation that the buffer was behaving as expected, i.e. uniform hydration from the rock contact inwards and closure of all gaps/joints, together with confirmation of sensor responses (Enresa 2006a). Since then, greater emphasis has been placed on process understanding and model development. The extension of the experiment timescale from an initial 3 years to now over 15 years has allowed a stronger focus and provided additional information particularly regarding saturation at low hydraulic gradients and geochemical processes.

#### THM understanding and impact of the transient state on final properties

While existing models have been "able to capture the main phenomena involved as well as their interactions" (Gens et al. 2009), the significance of longer-term effects relevant to late-time saturation such as thermo-osmosis, the double structure of compacted bentonite and possible hydraulic gradient thresholds could not be confirmed. Therefore, questions concerning the timing of achieving full saturation remain.

The expected development of a gradient in dry density within the buffer was confirmed by partial dismantling (Gens et al. 2009). Density ranged from 1.45 Mg/m<sup>3</sup> (close to the rock) to 1.7 Mg/m<sup>3</sup> (near the heater). The extent to which density will homogenise when temperature reduces and saturation is complete is uncertain. Data from the dismantling in 2015 should provide important further evidence.

#### Chemical understanding from excavation – characterising geochemical impacts and its potential to affect THM behaviour

FEBEX provides a unique opportunity to study geochemical processes within the buffer over many years. Models of THMC processes in the buffer (Samper et al. 2008a, Zheng et al. 2011) capture some aspects of system evolution over the 5 years of emplacement (1997 – 2002) prior to excavation of Heater # 1 but deviate from observations at the interfaces with rock and heater. Further data from a period of over 15 years would significantly extend the dataset. Of particular interest are iron/bentonite reactions (Samper et al. 2008c), which can be studied at the contact of the buffer with the liner, corrosion probes and sensors.

**Overall summary**

One can conclude that the impact of FEBEX has extended beyond the objectives of the original experiment and has:

- demonstrated the value of large-scale experiments in testing and refining disposal concepts
- provided a model for a significant number of experiments at real or near-real scale
- been used extensively as a dataset to support model development within FEBEX, DECOVALEX and other programmes



## 5 Conclusions and recommendations

The FEBEX In Situ and Mock-up Tests have provided, and are still providing, a unique insight into the EBS evolution at a realistic scale and over a time frame covering a significant part of the early EBS evolution in a repository. Although initiated over 15 years ago, FEBEX meets the current need to demonstrate the functioning and performance of complete repository components at the 1:1 scale under natural conditions.

### 5.1 The In Situ and Mock-up Tests

Concerning the In Situ Test, "after 15 years of continuous operation it is a still reliable installation, and both the heater and the instrumentation show no signs of ageing that could anticipate operation problems in the short term" (AITEMIN 2012). So while the FEBEX In Situ Test remained in good operational condition, it appears that in any reasonable timescale:

- changes in the state of the buffer were very slow and were unlikely to provide significant new information
- there was little prospect of achieving near full saturation (~ 99 %) throughout the buffer if the current operational conditions were maintained

Dismantling will provide a wealth of information on the state of the buffer (within the bentonite and at interfaces with the plug and liner), corrosion and microbial activity (although the existence/distribution of aerobic/anaerobic conditions needs to be determined). The value of this dismantling data to the experiment partners, given current timescales, outweighed any benefit from the continued operation. The "added value of continuing [the] experiment has to be balanced against information needs at specific occasions" (SKI 2004) and it was decided to switch off the remaining heater and start dismantling in 2015.

With the dismantling of the In Situ Test in 2015, the role of the Mock-up needs to be considered. The Mock-up instrumentation and heaters are in good condition and could continue to operate for several years. The Mock-up is particularly well placed to:

- refine the understanding of coupled processes and provide a test dataset for models
- provide further information on porewater geochemistry of the buffer and possible corrosion

Although continued higher temperatures favour corrosion, potentially providing more information if the Mock-up is dismantled, the observed stabilisation in saturation suggests that information from the Mock-up sensor data will not be able to discriminate between the different candidate hypotheses (e.g. thermal osmosis vs. influence of double structure) unless thermal boundary conditions are changed.

### 5.2 Detailed process understanding

#### 5.2.1 EBS

The EBS has largely performed as expected. The major processes and couplings affecting the buffer saturation during the initial thermal period had been identified prior to the start of the experiment. Buffer inhomogeneity due to construction has in fact played a smaller role than expected and a relatively uniform axisymmetric thermal, saturation and stress response controlled by distance from the heater has been observed. This is most obvious in data from the Mock-up and in the data from partial dismantling of the In Situ Test.

Much of the buffer in both the In Situ and Mock-up Tests is saturated and significant swelling pressures have developed throughout the greater part of the buffer. The low permeability of the saturated bentonite close to the rock ensures a slow saturation and inhomogeneity in rock properties have no influence on buffer saturation. Density gradients within the buffer have developed due to swelling on hydration and drying and shrinkage near the heater. These density gradients (following an axisymmetric pattern) are evident in the dismantling data, were reproduced in equivalent laboratory tests (Villar et al. 2012), and are as predicted by coupled models (Gens et al. 2009).

The role of 2<sup>nd</sup> order processes and couplings on saturation have become more important as hydraulic gradients have reduced and have potentially been highlighted by the application of constant temperature/power boundary conditions that are not representative of the expected conditions in a repository. The processes/couplings considered were:

- thermal osmosis
- threshold gradients for flow within the bentonite
- the influence of porosity structure evolution of the bentonite

Partial dismantling provided observation of some changes in buffer mineralogy and porewater chemistry related to the flux of water from the geosphere and redistribution of moisture within the buffer.

The effects of interactions between EBS components during saturation have also been observed under realistic conditions. Data are currently available for a 15-year period and dismantling will extend this to 18 years. An open issue is the existence of aerobic conditions within the buffer and its influence on corrosion and microbial processes.

### 5.2.2 Modelling

THM modelling within FEBEX has demonstrated its capability with regard to the prediction of the evolution of large-scale systems based on laboratory characterisation of the buffer, but has also identified the limits in its ability to discriminate between additional processes which ultimately determine the final part of the saturation process.

Progress is now needed with regard to process understanding. Targeted smaller-scale experiments and associated modelling are likely to provide the best way forward. Once this is achieved, the large-scale test dataset can be revisited.

The availability of a final dataset from the In Situ Test, together with data from supporting laboratory programmes and an extended dataset from the Mock-up provide an opportunity to make a synthesis regarding the capability of the "standard THM model" and its developments. One part of such a synthesis should be the development of a better understanding of the sensitivity of the models to key parameters (e.g. saturated bentonite permeability) and assumptions (see Johnson et al. 2008). The large-scale test dataset will also continue to be of great value in providing an opportunity to benchmark new THM approaches.

A significant improvement in THC/THMC modelling of the clay barrier has been achieved during the FEBEX project. THC/THMC codes were developed during the course of the project which could handle the observed thermo-hydro-geochemical couplings and account for the most relevant features of the THC conceptual model. THC/THMC models were constructed using data provided by a wide range of small-scale lab tests, together with thermal and hydrodynamic

data from the Mock-up and In Situ Tests and geochemical data from the partial dismantling. The ability of THC models to reproduce most of the observed patterns under a range of conditions increases confidence in their application. The final dataset from the In Situ Test now provides an opportunity to test the predictive capability of these models.

The majority of the THC/THMC analysis effort has been devoted to constructing thermo-hydro-geochemical models for the main geochemical processes controlling the geochemical evolution of the clay barrier in terms of major ion composition, pH and alkalinity. There are additional processes relevant for performance assessment, such as redox reactions and the interactions of corrosion products, which were not addressed within the FEBEX project.

In summary, FEBEX has provided a significant focus for demonstrating the predictive capability of THM models and for the continuing development of both, THM and THMC models.

### 5.2.3 Geosphere

While the rock at the FEBEX site shows the spatial variability that typifies many crystalline sites with highly localised fluid flow (Berkowitz 2002, Neuman 2005), the interaction between geosphere and EBS during FEBEX has been relatively easily understood and can largely be represented by homogeneous representations of the host rock (Alonso et al. 2005). The lack of significant geosphere influence on buffer saturation is due to:

- absence of very high inflow locations that might cause localised erosion or piping
- relatively high granite matrix conductivity ( $\sim 10^{-11}$  m/s) that has ensured that saturation is controlled by the bentonite (see Gens et al. 2002)

Similarly, disturbances in the geosphere (drilling and opening of nearby boreholes) have had only very limited, if any, effect on the EBS.

The homogeneity in water uptake from the geosphere observed at FEBEX may not be the case at sites where the host rock matrix permeability is significantly lower.

## 5.3 Conclusions for performance of the EBS system

The development of a low permeability, highly saturated outer layer of the buffer with significant swelling pressures and the absence of any indication of preferential flow demonstrates that the buffer will achieve the required performance over time as saturation increases. The time for saturation of the large-scale tests under a thermal gradient may be longer than anticipated by application of "standard THM models", but evidence from smaller-scale test suggest that uniformly highly saturated conditions can be achieved (Villar et al. 2012).

While construction joints appear to have quickly sealed and have little influence on the saturation, gradients in dry density have developed within the buffer. These gradients follow an axisymmetric distribution influenced by the development of swelling pressure due to hydration. This pattern is further modified by the influence of the heaters. The extent to which these gradients will homogenise over time cannot be addressed by the large-scale tests.

Evidence of significant corrosion and microbial activity after 5 years is limited to one instrument section, where high humidity (distant from the heater) and the presence of sulphate reducing bacteria (SRB) in the bentonite resulted in corrosion damage.

Evidence of mineralogical changes within the buffer after 5 years are of limited importance, with no macroscopic mineralogical change and near constant global chemistry (Enresa 2006b).

It is expected that results from the final excavation in 2015, after 18 years of chemical impacts taking place, will provide more evidence regarding the corrosion and the chemical processes affecting the EBS.

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- Zheng, L., Samper, J., Montenegro, L. & Fernández, A.M. (2010): A Coupled THMC Model of a Heating and Hydration Laboratory Experiment in Unsaturated Compacted FEBEX Bentonite. *Journal of Hydrology* 386/1-4, 80-94.
- Zheng, L., Samper, J. & Montenegro, L. (2011): A Coupled THC Model of the FEBEX in Situ Test with Bentonite Swelling and Chemical and Thermal Osmosis. *Journal of Contaminant Hydrology* 126/1-2, 45-60, doi:10.1016/j.jconhyd. 2011.06.003.



## Appendix A Selected references for FEBEX projects, In Situ Test models and Mock-up Test models

Tab. A-1: Key reports for FEBEX I, FEBEX II, DECOVALEX III and NF-PRO.

Report number	Full reference
FEBEX I	
PT 1998-01	Enresa (1998): FEBEX. Pre-operacional stage. Summary report. Enresa Report PT 1998-01. <sup>26</sup>
PT 1998-09	Enresa (1998): FEBEX. Preoperational thermo-hydro-mechanical (THM) modelling of the "in situ" test. Enresa Report PT 1998-09.
PT 1998-10	Enresa (1998): FEBEX. Preoperational thermo-hydro-mechanical (THM) modelling of the "Mock-up" test. Enresa Report PT 1998-10.
PT 1998-12	Enresa (1998): FEEX. Final design and installation of the "in situ" test at Grimsel. Enresa Report PT 1998-12.
PT 2000-01	Enresa (2000): FEBEX Project. Full-Scale engineered barriers experiment for a deep geological repository for high level radioactive waste in crystalline host rock. Enresa Report PT 2000-01.
FEBEX II	
PT 2002-04	Enresa (2002): Thermo-hydro-mechanical characterisation of a bentonite from Cabo de Gata. A study applied to the use of bentonite as sealing material in high level radioactive waste repositories. Enresa Report PT 2002-04.
PT 2003-09	Enresa (2003): Dismantling of the heater 1 at the FEBEX "in situ" test. Description of operations. Enresa Report PT 2003-09.
PT 2004-08	Enresa (2004a): FEBEX PROJECT. Post-mortem analysis: corrosion study. Enresa Report PT 2004-08.
PT 2004-09	Enresa (2004b): FEBEX PROJECT. THG laboratory experiments. Enresa Report PT 2004-09.
PT 2004-10	Enresa (2004c): FEBEX PROJECT. Final report on thermo-hydro-mechanical laboratory tests. Enresa Report PT 2004-10.
PT 2004-11	Enresa (2004d): FEBEX PROJECT. Post-mortem analysis EDZ assessment. Enresa Report PT 2004-11.
PT 2006-05-0	Enresa (2006a): Full-scale Engineered Barriers Experiment. Updated Final Report 1994-2004. Enresa Report PT 2006-05-0.
PT 2006-05-1	Enresa (2006b): FEBEX Project final report. Post-mortem bentonite analysis. Enresa Report PT 2006-05-1.
PT 2006-05-2	Enresa (2006c): FEBEX Project final report. Final report on the thermo-hydro-mechanical modelling. Enresa Report PT 2006-05-2.
PT 2006-05-3	Enresa (2006d): FEBEX Project final report. Final THG modelling report. Enresa Report PT 2006-05-3.

<sup>26</sup> Enresa reports are available from [www.enresa.es](http://www.enresa.es).

Tab. A-1: (continued)

<b>Report number</b>	<b>Full reference</b>
PT 2006-05-4	Enresa (2006e): FEBEX Project final report. Post-mortem analysis: instruments. Enresa Report PT 2006-05-4.
PT 2006-05-5	Enresa (2006f): FEBEX Project final report. Addendum sensors data report. In situ experiment. Enresa Report PT 2006-05-5.
PT 2006-05-6	Enresa (2006g): FEBEX Project final report. Addendum sensors data report. Mock-up Test. Enresa Report PT 2006-05-6.
EUR 21922	European Commission (2005): Full-Scale Engineered Barriers Experiment for a Deep Geological Repository for High-Level Waste in Crystalline Host Rock – Phase II: FEBEX II. European Commission Report Number EUR 21922. <sup>27</sup>
DECOVALEX III	
SKI 2005:20	Alonso, E.E. & Alcoverro, J. (2005): DECOVALEX III PROJECT: Modelling of FEBEX In-Situ Test. SKI Report 2005:20, Stockholm, Sweden. <sup>28</sup>
NF-PRO	
EUR 23730	European Commission (2008): Understanding and Physical and Numerical Modelling of the Key Processes in the Near Field and their Coupling for Different Host Rocks and Repository Strategies (NF-PRO): Final Report. European Commission Report Number EUR 23730.

<sup>27</sup> European Commission reports are available at <http://cordis.europa.eu/>.

<sup>28</sup> SKI reports are available at <http://www.stralsakerhetsmyndigheten.se/>.

Tab. A-2: Selected references for In Situ Test Models (shaded models include THG/THMC coupling).

Reference	Full reference
Enresa 1998	Enresa (1998): FEBEX. Preoperational thermo-hydro-mechanical (THM) modelling of the "in situ" test. Enresa Report PT 1998-09.
Gens et al. 1998	Gens, A., Garcia-Molina, A.J., Olivella, S., Alonso, E.E. & Huertas, F. (1998): Analysis of a full scale in situ test simulating repository conditions. <i>International Journal for Numerical and Analytical Methods in Geomechanics</i> 22/7, 515-548.
Sánchez & Gens 2002	Sánchez, M. & Gens, A. (2002): Second report on THM modelling results. FEBEX II, Enresa Report: 70-UPC-L-5-011.
Alonso et al. 2005	Alonso, E.E., Alcoverro, J., Coste, F., Malinsky, L., Merrien-Soukatchoff, V., Kadiri, I., Nowak, T., Shao, H., Nguyen, T.S., Selvadurai, A.P.S., Armand, G., Sobolik, S.R., Itamura, M., Stone, C.M., Webb, S.W., Rejeb, A., Tijani, M., Maouche, Z., Kobayashi, A., Kurikami, H., Ito, A., Sugita, Y., Chijimatsu, M., Börgesson, L., Hernelind, J., Rutqvist, J., Tsang, C.-F. & Jussila, P. (2005): The FEBEX benchmark test: case definition and comparison of modelling approaches. <i>International Journal of Rock Mechanics and Mining Sciences</i> , 42/5-6, 611-638, doi:10.1016/j.ijrmms.2005.03.004.
Rutqvist & Tsang 2004	Rutqvist, J. & Tsang, C.-F. (2004): A fully coupled three-dimensional THM analysis of the FEBEX in situ test with the ROCMAS Code: Prediction of THM behavior in a bentonite barrier. <i>In</i> : Stephansson, O. (ed.): <i>Coupled Thermo-Hydro-Mechanical-Chemical Processes in Geo-Systems: Fundamentals, Modelling, Experiments and Applications</i> . Elsevier Geo-Engineering Book Series, 143-148.
Zheng et al. 2005	Zheng, L. & Samper, J. (2005): Inverse problem of non-isothermal multiphase flow and reactive transport in deformable porous media. VII Jornadas de Investigación en la Zona no Saturada de Suelo, ZNS'05. La Coruña, Spain, 307-312.
Enresa 2006c (PT 2006-05-2)	Enresa (2006): FEBEX Project final report. Final report on the thermo-hydro-mechanical modelling. Enresa Report PT 2006-05-2.
Enresa 2006d (PT 2006-05-3)	Enresa (2006): FEBEX Project final report. Final THG modelling report. Enresa Report PT 2006-05-3.
Samper et al. 2008	Samper, J., Zheng, L., Montenegro, L., Fernández, A.M. & Rivas, P. (2008): Coupled thermo-hydro-chemical models of compacted bentonite after FEBEX in situ test. <i>Applied Geochemistry</i> 23/5, 1186-1201, doi:10.1016/j.apgeochem.2007.11.010.
Zheng et al. 2008	Zheng, L., Samper, J. & Montenegro, L. (2008): Inverse hydrochemical models of aqueous extract experiments. <i>Physics and Chemistry of the Earth</i> 33/14, 1009-1018.
Gens et al. 2009	Gens, A., Sánchez, M., Guimarães, L.D.N., Alonso, E.E., Lloret, A., Olivella, S., Villar, M.V. & Huertas, F. (2009): A full-scale in situ heating test for high-level nuclear waste disposal: observations, analysis and interpretation. <i>Géotechnique</i> 59/4, 377-399, doi:10.1680/geot.2009.59.4.377.

Tab. A-2: Cont.

Reference	Full reference
Francois & Laloui 2009	Francois, B. & Laloui, L. (2009): Behaviour of an engineered clay barrier for a nuclear waste isolation system. In: Int. Conf. on Computational Methods for Coupled Problems in Science and Engineering Coupled Problems 2009, 1-4.
Buil et al. 2010	Buil, B., Gómez, P., Peña, J., Garralón, A., Turrero, M.J, Escribano, A., Sánchez, L. & Durán, J.M. (2010): Modelling of bentonite–granite solutes transfer from an in situ full-scale experiment to simulate a deep geological repository (Grimsel Test Site, Switzerland). Applied Geochemistry 25/12, 1797-1804, doi:10.1016/j.apgeochem.2010.09.003.
Gens et al. 2010	Gens, A., Guimarães L.D.N., Olivella, S. & Sánchez, M. (2010): Modelling thermo-hydro-mechano-chemical interactions for nuclear waste disposal. Journal of Rock Mechanics and Geotechnical Engineering 2010/2, 97-102, doi:10.3724/SP.J.1235.2010.00097.
Zheng et al. 2011	Zheng, L., Samper, J. & Montenegro, L. (2011): A coupled THC model of the FEBEX in situ test with bentonite swelling and chemical and thermal osmosis. Journal of contaminant hydrology 126/1-2, 45-60, doi:10.1016/j.jconhyd.2011.06.003.
Sánchez et al. 2012	Sánchez, M., Gens, A. & Guimarães, L. (2012): Thermal-hydraulic-mechanical (THM) behaviour of a large-scale in situ heating experiment during cooling and dismantling. Canadian Geotechnical Journal 49/10, 1169-1195, doi:10.1139/T2012-076.
Olivella et al. 2012	Olivella, S., Mokni, N. & Gens, A. (2012): FEBEXe Project: Final Report, Universitat Politècnica de Catalunya, Barcelona, Spain.
Dupray et al. 2013	Dupray, F., François, B. & Laloui, L. (2013): Analysis of the FEBEX multi-barrier system including thermoplasticity of unsaturated bentonite. International Journal for Numerical and Analytical Methods in Geomechanics 37/4, 399-422, doi:10.1002/nag.

Tab. A-3: Selected references for Mock-up Test models (shaded models include THG/THMC coupling).

<b>Reference</b>	<b>Full Reference</b>
Enresa 1998	Enresa (1998): FEBEX. Preoperational thermo-hydro-mechanical (THM) modelling of the "in situ" test. Enresa Report PT 1998-09.
Sánchez et al. 2004	Sánchez, M., Gens, A. & Olivella, S. (2004): Thermo-hydro-mechanical modelling of low permeability media using a double-porosity formulation. <i>Mecanica Computacional XXIII</i> (November), 733-754.
Enresa 2006c	Enresa (2006): FEBEX Project final report. Final report on the thermo-hydro-mechanical modelling. Enresa Report PT 2006-05-2.
Enresa 2006d	Enresa (2006): FEBEX Project final report. Final THG modelling report. Enresa Report PT 2006-05-3.
Zheng & Samper 2008	Zheng, L. & Samper, J. (2008): A coupled THMC model of FEBEX mock-up test. <i>Physics and Chemistry of the Earth, Parts A/B/C</i> 33, S486-S498, doi:10.1016/j.pce.2008.10.023.
Sánchez et al. 2010	Sánchez, M., Gens, A. & Olivella, S. (2010): Effect of thermo-coupled processes on the behaviour of a clay barrier submitted to heating and hydration. <i>Anais da Academia Brasileira de Ciências</i> 82/1, 153-68.
Sánchez et al. 2012	Sánchez, M., Gens, A. & Olivella, S. (2012): THM analysis of a large-scale heating test incorporating material fabric changes. <i>International Journal for Numerical and Analytical Methods in Geomechanics</i> 36/4, 391-421, doi:10.1002/nag.1011.



## Appendix B Investigations and Evaluation of Slowing of Hydration in Mock-up Test

By M. Villar & P.L. Martín

### B.1 Investigations 2000 – 2001

#### B.1.1 Observed decrease in the water-inlet rate

The decrease in the water inlet rate to the Mock-up was first observed around day 800, as shown in Fig. B-1. Several possibilities were proposed and analysed to explain this behaviour.

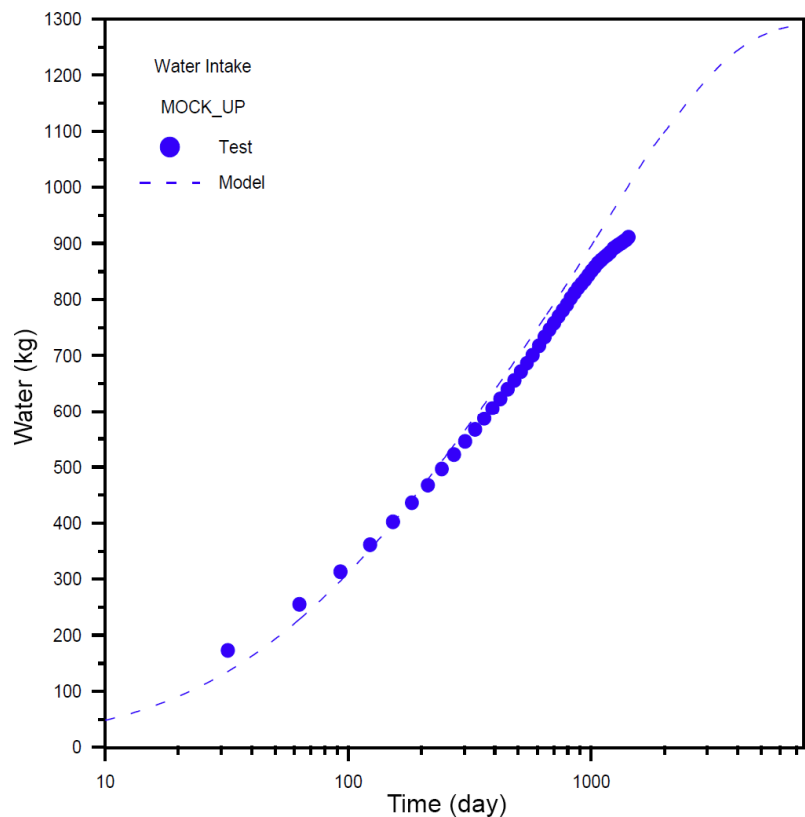


Fig. B-1: Water inlet: measurement vs. model prediction (OBC) for the Mock-up Test.

#### Clogging of the water injection nozzles

Due to the design of the injection nozzles and the associated system of filters, the possibility of clogging at these points by clay was not considered likely. The system is composed (Fig. B-2) from the outer to the inner part of two sintered metal filters inserted into the nozzle (MOTT Industrial, SS316L,  $\varnothing$  6.25 mm, pore size 60 – 100  $\mu$ m), a mesh disk (SS316L,  $\varnothing$  20 mm, n<sup>o</sup> 100, aperture 0.15 mm) and a geotextile disk (EXXON TERRAM 4000,  $\varnothing$  25 mm,). Both disks were glued to the structure.

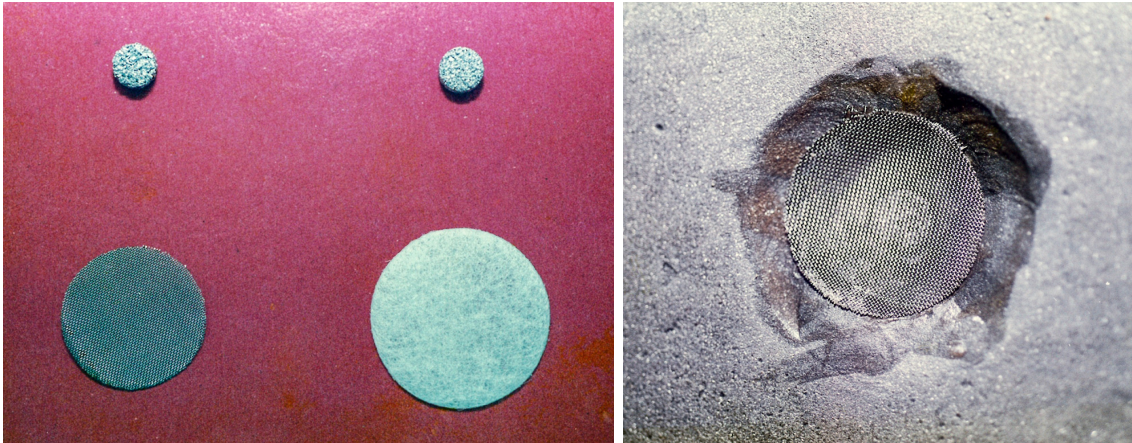


Fig. B-2: System of filters in the injection nozzles for the Mock-up Test.

### **Clogging of the geotextile layer**

Four layers of geotextile cover the inner surface of the structure (Fig. B-3) to assure a distribution as homogeneous as possible of the injection water. The properties of the geotextile (EXXOM TERRAM 4000, thermally bonded non-woven, 70 % polypropylene, 30 % polyethylene) were verified in the laboratory (Villar & Martin 1997) under pressures of up to 5 MPa. Water permeability, both parallel and perpendicular to the layers (around  $10^{-8}$  m/s) and consolidation (more than 50 % volume reduction, non-recoverable) were measured. Temperature (60 °C) did not seem to affect the geotextile properties.



Fig. B-3: Installation of geotextile layers in the Mock-up Test structure prior to bentonite emplacement.

To check if clogging of the geotextile layer had occurred, all 48 valves at the injection points were closed, except two which were located in different hydration rings. Water was injected in one and collected in the other. The amount of water injected as measured by the weighing system was equivalent to the amount of water recovered. This demonstrated that the geotextile layer had high transmissivity under the operating conditions.

In fact, the measured water flow between the hydration rings was much higher than the water flow into the whole EBS as expected from the difference in the water permeability values of the two materials: the geotextile has a permeability six orders of magnitude higher.

**System (test) geometry**

Due to the geometry of the test, the surface of the hydration front is smaller, as the wetting front goes inwards, which reduces the water intake potential.

**B.1.2 Observed decrease of the water pressure**

A decrease of the water pressure values in locations connected with the geotextile layers was also detected (Fig. B-4). It began around day 640. Pressures reduced from 5 to 1 bar. The observed pressure decrease is explained by bentonite intrusion into the gaps at the input/output locations in the structure. The bentonite intrusion clogs the active zone of the sensors near these points.

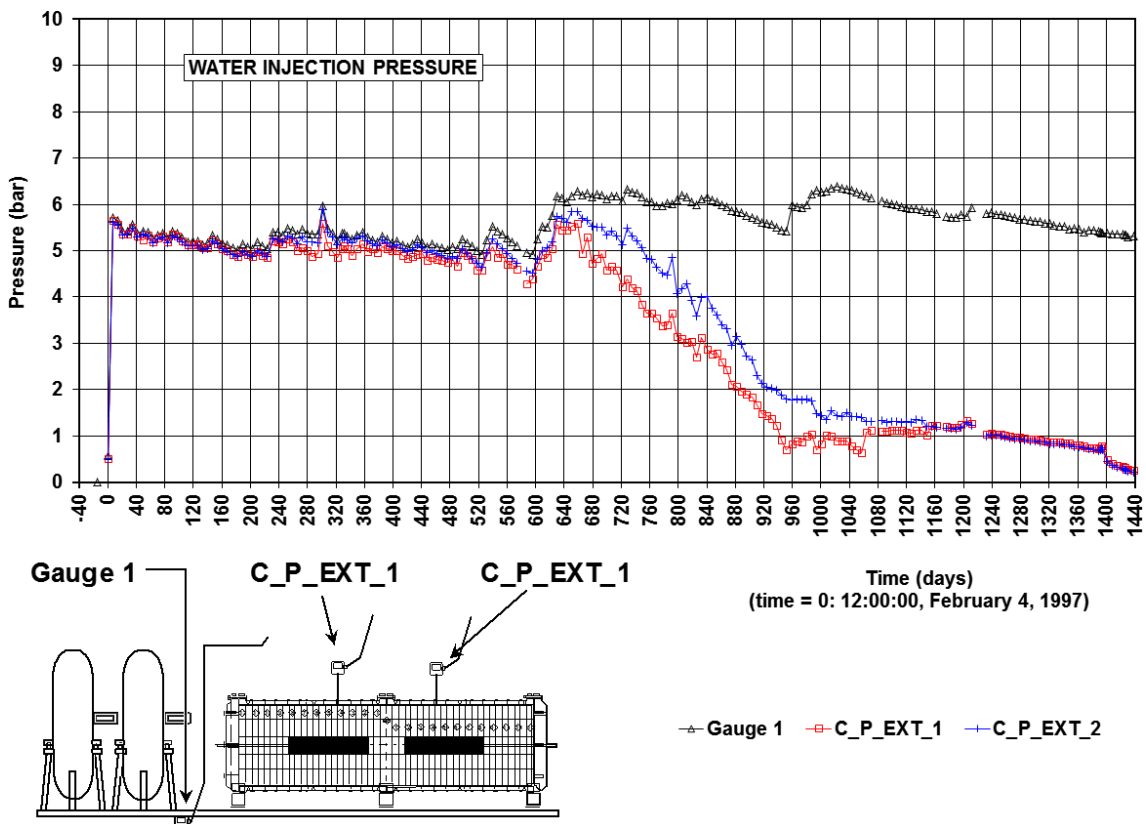


Fig. B-4: Water injection pressure (Mock-up Test).

The geotextile layers were perforated at the input/output locations for the cables, so that at these locations the bentonite is in contact with the structure (Fig. B-5) over a small area (around  $\varnothing$  20 mm). The minimum distance from these perforated points to the injection points is 0.25 m. This area is completely covered by the four layers of geotextile compressed by the bentonite swelling. Thus, the possibility of bentonite extruding through the sensor inlets and moving to the injection points is not considered plausible.

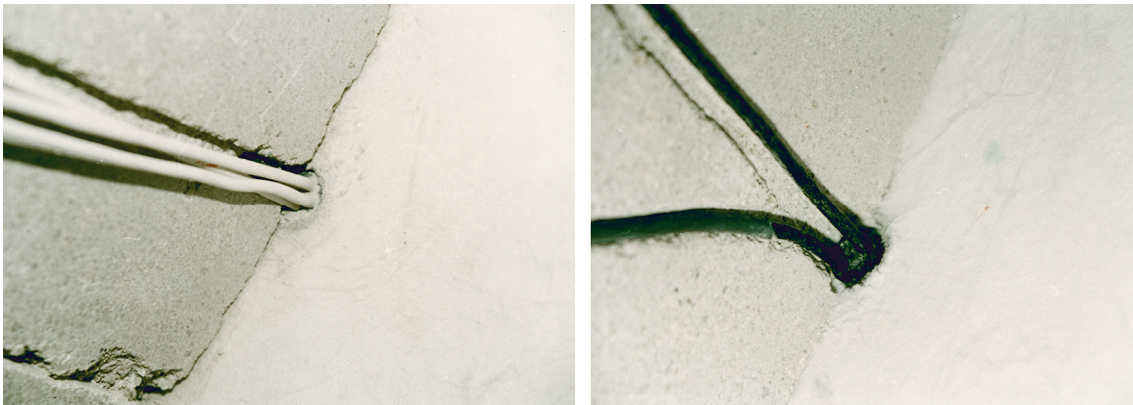


Fig. B-5: Mock-up Test input/output cable locations prior to installation of geotextile.

### B.1.3 Observed decrease of the relative humidity

The slight decrease of relative humidity occurred simultaneously with the pressure decrease and several potential causes were analysed:

#### Gas concentration in the barrier

Gas concentration in the barrier that cannot be dissipated could reduce the progress of the hydration front. Pressurised gas would come from the initial air contained in the porosity of the barrier, from canister corrosion, bacterial activity, or from the hydration circuit (pressurised  $N_2$ ). However, the fluid pressure sensors that worked correctly during the overheating episode did not indicate any significant gas pressures in the barrier. So, this cause was ruled out.

#### Anomalous function of the sensors

The evolution of the relative humidity sensors was homogeneous, following similar patterns among them, which indicates that they were working properly. However, an aging process affecting the sensors could not be discarded.

### B.1.4 Dynamics of barrier hydration

Several factors affect the dynamics of the barrier hydration:

- **Injection pressure.** The effect of injection pressure is insignificant compared to the high suction of the partially saturated bentonite. At the time when the hydration rate was observed to decrease, the suctions measured close to the hydration surface were well above the injection pressure (10 MPa vs. 0.5 MPa). Currently, the suctions corresponding to

relative humidity values slightly higher than 99 % are also above the injection pressure (0.69 MPa vs. 0.5 MPa).

- **Bentonite suction.** It is the main driving force for hydration of the partially saturated barrier. This is true in the zones around the heaters, but it is also important in the almost saturated external zones. As explained above, values of suction similar or higher than those of the water injection can be found in the region of the external part of the barrier considered as "fully-saturated".
- **Bentonite permeability.** In the beginning, permeability was very low but, as the hydration progresses, two opposite processes occur: the relative permeability increases with the increasing saturation and the intrinsic permeability decreases due to the redistribution of the porosity (macro-porosity transforms into micro-porosity). After a first expansion of the outer bentonite, the development of the swelling pressure in the inner zones of the barrier compresses the outer saturated bentonite again, increasing its dry density and, consequently, decreasing its intrinsic permeability.

## B.2 More recent work including modelling

### B.2.1 Differences between In Situ and Mock-up Tests

Even in the case that "coupled diffusive" processes were exclusively responsible for the energy and mass transfer, the geometric factors are also very important.

1. The external/internal radius ratio of the barrier is much higher in the Mock-up than in the In Situ Test (5 vs. 2.5), which means the behaviour of the Mock-up diverges more from a "plane-sheet" (linear geometry) behaviour than the In Situ Test.
2. The differences between the external temperatures (Mock-up vs. In Situ Test) and the internal temperature (experiment control temperature), along with the above geometric factors result in a slightly different temperature distribution across the barrier in the two tests.
3. The interface between the heater (impervious) and the bentonite is direct in the Mock-up. In the In Situ Test there is a liner along the centre of the bentonite buffer that provides an important void space along the whole experiment for mass transport (with probable piping of gases and water vapour). This gap could be observed in the pictures from the first dismantling.
4. The Mock-up is only hydrated through the curved surface of the confining structure. While the ends of the confining structure are impervious, the In Situ Test is also hydrated through the porous concrete plug and the end of the gallery. The relevance of this difference is given by the existence of a longitudinal liner in the In Situ Test that could favour water migration along its surface (see above).
5. The initial flooding of the Mock-up Test to seal the gaps among blocks provided a homogeneous hydration surface and eliminated the preferential pathways for water and vapour into the bentonite barrier. These preferential paths were present in the In Situ test during an initial period but had largely healed after 5 years (at partial dismantling).
6. There are also significant differences in the overall dry density (Mock-up 1.65 vs. In Situ 1.6 Mg/m<sup>3</sup>) that affect the hydraulic conductivity through porosity (and suction).
7. The above points indicate that the processes in the Mock-up was influenced by the limits of the bentonite barrier system (heater walls) significantly before the In Situ Test. The consequence is the slowdown of the processes inside the buffer.

### **B.2.2 Geotextile considerations**

After Palmeria & Gardoni (2000), the factors that could affect the geotextile function are the magnitude of swelling pressure of bentonite against the geotextile, the hydraulic gradient along the geotextile, the physical disturbances on the geotextile (bending, folding, twisting, and crimping), the installation disturbance (gas bubbles), and the permeability of geotextile by intrusion of fine particles termed as filtration and clogging. Physical and installation disturbances can be discarded.

The swelling pressure in the external ring has remained in a narrow range for a long time, hence the progressive compaction of the geotextile due to bentonite pressure can be ruled out.

The initial flow is controlled by the hydraulic gradient and properties of the soil (in this case the bentonite), not by the geotextile-soil system (Gardoni & Palmeria 2002). If we consider that the saturated surface of the compacted bentonite is almost impervious to water, the hydraulic gradient along the geotextile layers must be constant and very low, with no influence on the hydraulic behaviour of the geotextile.

So, the only factor to be considered would be the changes in geotextile permeability due to the initial consolidation phase in the short term, and by filtration and clogging in the long term. The latter process was discarded after the experimental check described in the previous section. Even in the case that the geotextile permeability had reduced during the experiment, it would still be much higher than that of the bentonite, since the initial difference between the two material permeabilities is six orders of magnitude.

### **B.2.3 Summarised from Villar et al. (2012) and Sánchez et al. (2012a)**

#### **From Villar et al. (2012)**

Villar et al. (2012) compared different long-term experiments to establish that the rate of hydration of the barrier depends on the bentonite and surrounding media hydraulic properties (that is, water availability), waste temperature and buffer thickness and geometry.

Furthermore, in a large-scale in situ experiment that examined isothermal water inflow from the surrounding granitic rock into highly compacted, unsaturated buffer material, Dixon et al. (2002) observed that, after 6.5 years of operation, the water uptake had been much lower than initially expected. The simulation of this experiment, taking into account the expansion of the microstructure of the bentonite as the material saturated, matched with much greater accuracy both the pattern and rate of water uptake (Thomas et al. 2003).

#### **From Sánchez et al. (2012)**

Several studies were carried out to explore possible phenomena that could cause the unexpected barrier behaviour (slowdown in the FEBEX Mock-up Test). Firstly, a wide-ranging sensitivity study found it impossible to obtain a set of constitutive laws and materials parameters (with physical meaning) that led to predictions consistent with the observations. Secondly, it was found that whether the experiment was airtight or not had no influence on the results. Thirdly, the hydration system of the experiment was examined and it was experimentally confirmed that there was no obstruction in the hydration system or geotextile and that the water intake was nearly uniform over the entire hydration front. Similar observations in other experiments support a genuine slowing down of hydration. For example, a lower level of saturation, com-

pared with the expected one, has been observed in the large-scale ITT test performed in the Canadian underground laboratory near Winnipeg. Thomas et al. (2003) concluded that "standard THM models" were not able to capture the slow hydration observed in the experiment.

Experimental evidence indicates that the behaviour of expansive clays under confined hydration is more complex than the conventional THM model used in the numerical analysis. Instead of a progressive increment of the water permeability in external zones of the barrier as saturation goes on, a progressive occlusion of the macro-pores has been observed in the laboratory leading to potentially large reductions in saturated water permeability.

The evolution of the clay fabric (macro- and micro-porosity) is controlled by the changes in the main variables of the problem (displacements, temperature and suction), which are considered in a fully coupled way in the models described by Sánchez et al. (2012a). According to the model results, as the barrier hydration progresses, the macro-pores available to the liquid flow suffer a progressive reduction. This is due mainly to microstructural swelling under confined conditions. As a consequence, the full saturation of the barrier is drastically delayed. This phenomenon affects especially the zones close to the heater, because the reduction of the permeability in the zones close to the hydration front reduces the liquid flow supply to the internal zones, which have been subjected to heating-induced drying.

### **B.3 Conclusions**

The checks performed when the first anomalous behaviour was observed did not indicate any problem in the hydration system. The capacity to supply water to the experiment (via the geotextile) was very much higher than the saturation rate of bentonite.

The differences between the Mock-up and In Situ Test include geometrical, material and operational factors that affect the behaviour of each test. It is also necessary to include the different boundary conditions. Even if the geotextile permeability had reduced during the experiment, it would still be much higher than that of the bentonite since the initial difference between the two material permeabilities is six orders of magnitude.

The double structure model (Sánchez et al. 2012a) is able to simulate the type of hydration locking observed in the test, where significant zones of the barrier may remain in a partially saturated condition for a considerable period of time. However, other physical and chemical phenomena could also influence the slow hydration observed in the clay barrier.



## Appendix C UDC Summary of THC/THmC Modelling

By J. Samper & L. Montenegro

### C.1 Introduction

One of the objectives of the FEBEX project was the study, identification and modelling of the possible geochemical alterations that could occur in the engineered barrier due to the combined effect of high temperatures and water flow. To this purpose, a detailed and extensive laboratory programme was carried out in order to provide thermo-hydro-geochemical (THC) parameters and identify the processes triggered by temperature and water flow. Inasmuch as geochemical processes are linked and affected by thermal and hydrodynamic processes, identification and modelling of geochemical alterations requires a coupled THC/THmC analysis. In complex systems such as the clay barrier, this analysis must be performed with numerical models using appropriate THC codes.

This appendix presents the UDC THC/THmC modelling of laboratory experiments, and Mock-up and In Situ Tests. These THC/THmC models developed by UDC rely on flow, thermal, transport and geochemical conceptual models. Multicomponent solute transport mechanisms include advection, molecular diffusion, and mechanical dispersion. Chemical reactions considered in the models include: aqueous complexation, acid-base, calcite, quartz/chalcedony and gypsum/anhydrite dissolution/precipitation,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  cation exchange, and proton surface complexation. Codes employed to solve the THC numerical models include: CORE: CORE<sup>2D</sup> V4 (Samper et al. 2003, 2011), FADES-CORE (Juncosa 2001), INVERSE-CORE<sup>2D</sup> (Dai & Samper 2004) and INVERSE-FADES-CORE (Zheng & Samper 2004, Zheng et al. 2005). These numerical tools have been used to:

1. Interpret laboratory tests for parameter estimation
2. Interpret laboratory tests to identify relevant geochemical processes
3. Predict the transport patterns of artificial tracers in both the Mock-up and In Situ Tests
4. Predict the THC performance of the engineered barrier for the Mock-up and In Situ Tests
5. Test THC predictions with dismantling data from around Heater # 1 of the In Situ Test

#### C.1.1 Thermo-hydro-geochemical conceptual models

Conceptual THC/THmC models have been based on the THM processes outlined in Gens et al. (2009) as:

- Thermal:
  - Heat conduction and advection<sup>29</sup> (mobile phases)
  - Latent heat of phase changes
- Hydraulic:
  - Liquid and gas flow
  - Water evaporation and condensation
  - Binary diffusion of air and water

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<sup>29</sup> Heat advection is included in the formulation but it turns out to be negligible in this application.

- Dissolution of air in water
- Diffusion of air in water
- Mechanical:
  - Deformation due to changes in stress, suction, pore pressure & temperature
  - Deformation of both solid skeleton and constituent phases

The fluid and thermal fluxes control the mixing of the bentonite porewater and granite porewaters and their reactions with the bentonite minerals.

Multiple conceptual models for the bentonite porewater were considered on the basis of the datasets used (obtained from squeezing tests or from aqueous extracts):

CGM-0: Squeezing data (Samper et al. 2001)

CGM-Ciemat: Squeezing and aqueous extraction data (Fernández et al. 1999, 2001)

CGM-1: Aqueous extraction data (Samper et al. 2005a)

CGM-2: Modified version of CGM-1 including squeezing data (Samper et al. 2005a)

The models reflect different balances between the two porewater datasets. The datasets are affected by the artefacts induced by the two methods: squeezing and aqueous extraction.

Consideration of the influence of mechanical processes has focussed on swelling and associated changes in porosity via simplified models (Zheng et al. 2011). Transport mechanisms include: advection, molecular diffusion and mechanical dispersion. The chemical processes considered in the models have developed over time to include: aqueous complexation, acid-base reactions, mineral dissolution/precipitation, cation exchange and surface complexation (Zheng et al. 2011). Additional processes regarding possible CO<sub>2</sub> degassing have also been suggested.

## **C.2 THC/THmC modelling of laboratory tests**

Many different types of laboratory experiments were performed within FEBEX projects to provide support to the Mock-up and In Situ Tests. The success of the FEBEX project relied to a large extent on the extensive laboratory programme. Some of these laboratory tests including squeezing and aqueous extract tests (AET) at different durations and at different S/L ratios, AET of samples from the In Situ Test, and laboratory heating and hydration experiments on thermo-hydraulic cells (permeation test and CT23 cell) have been modelled as part of the development of THC/THmC models. Numerical interpretation has been performed by UDC with close interaction with CIEMAT researchers.

### **C.2.1 Modelling squeezing and AET at different durations and S/L ratios**

One of the major uncertainties in the geochemical conceptual model is the chemical composition of the FEBEX bentonite porewater (at 14 % water content). However, obtaining reliable data for clay porewater chemistry is a difficult task. Squeezing at high pressures and aqueous extracts, which have been used to obtain porewater from the compacted FEBEX bentonite, may alter the water-clay system in several ways and introduce sampling artefacts in measured data. Squeezing at high pressures may induce oxidation and dissolution of accessory minerals of the bentonite, outgassing of CO<sub>2</sub>(g), and chemical fractionation (Sachi and Michelot 2000). Furthermore, squeezing does not allow extraction of porewater from bentonites with water contents

below 20 %. Therefore, the squeezing method cannot be used for characterising bentonite at ambient conditions with a water content of 14 %. For these conditions one must use the aqueous extract technique.

The aqueous extract technique provides a method to quantify the total content of soluble salts (Parker 1921) because it works with a low solid-to-liquid ratio. An 1:R aqueous extract test consists on adding to a mass M of clay sample a mass of distilled water equal to R times M. The mixture of solid and water is allowed to react during a period of time (usually 2 days). After that, liquid and solid phases are separated by centrifugation. Chemical analyses are performed on the supernatant solution. During the extraction, mineral dissolution of various soluble minerals (halite, carbonates and gypsum) as well as cation exchange processes take place which affect the concentrations of dissolved species. These processes complicate the interpretation of aqueous extract data.

Since laboratory techniques used to obtain bentonite porewater may alter the geochemical system and introduce sampling artefacts, indirect methods based on hydrogeochemical modelling are needed in order to infer the chemical composition of bentonite porewater. Different methods have been developed to model and interpret chemical analyses of FEBEX bentonite porewater obtained by AET performed by CIEMAT on intact FEBEX bentonite samples at the following 1:R ratios: 1:1, 1:2, 1:4, 1:8, 1:10 and 1:16 with distilled and granitic water (Fernández et al. 1999, 2001). Tests were also performed with different reaction times ranging from 2 to 30 days for a 1:4 ratio in order to evaluate the kinetics of mineral dissolution/precipitation. Results obtained from these tests (Samper et al. 2005a, 2005b, Enresa 2006a, 2006d) are compared to values derived from squeezing tests carried out by CIEMAT.

Initial bentonite porewater concentration was obtained by inverse hydrogeochemical modelling using the reactive transport code CORE<sup>2D</sup> (Samper et al. 2003). Starting with the initial chemical composition of bentonite porewater at a water content of 14 %, distilled water is added until the appropriate S/L ratio of the test is attained. Distilled water added to bentonite samples has a pH of 7 and the chemical concentration of all species is 10 – 20 mol/L. CO<sub>2</sub>(g) is fixed at atmospheric pressure (10<sup>-3.5</sup> bar).

The main conclusions of hydrogeochemical modelling of bentonite porewater chemistry obtained by aqueous extract and squeezing tests include:

- Model CGM-1 derived from aqueous extract data reproduces measured data of tests performed for durations up to 30 days. Most chemical species reach equilibrium before 10 days. Therefore, calcite and dolomite kinetics are rather fast. For the most part, this model fits measured data at different S/L ratios. However, it fails to reproduce the trend of bicarbonate, possibly due to changes in the CO<sub>2</sub>(g) pressure which are not considered in the model. Computed results with model CGM-1 show slight deviations for the 1:1 test for chloride, sodium and potassium. In general, this model cannot fit squeezing data.
- Model CGM-2 is able to fit simultaneously aqueous extract data and squeezing data, although it presents some clear deviations for sulphate.
- Measured data tend to reject the hypothesis of a constant pressure of CO<sub>2</sub>(g) during the tests.

### C.2.2 Inverse hydrochemical models of AET of the In Situ Test

Measured aqueous extract data from bentonite samples collected after dismantling of Heater # 1 in the In Situ Test have to be re-interpreted in order to infer porewater chemical composition of the sample because porewater chemistry changes significantly due to dilution and chemical reactions which take place during extraction.

Zheng et al. (2008) presented an inverse hydrochemical model to estimate porewater chemical composition from measured water content, aqueous extract, and mineralogical data. The inverse method to interpret AET provides a comprehensive way to estimate the chemical composition of clay porewater because it accounts for a wide range of chemical processes such as: acid-base, redox, aqueous complexation, mineral dissolution/precipitation, gas dissolution/ex-solution, cation exchange and surface complexation reactions, all of which are assumed to take place at local equilibrium. It has been solved with INVERSE-CORE<sup>2D</sup> (Dai & Samper 2004) and tested with bentonite samples from the FEBEX In Situ Test taken at different radial distances along Sections 19 and 29 located at both edges of Heater # 1. The inverse model reproduces most of the measured aqueous data except bicarbonate and provides an effective, flexible and comprehensive method to estimate porewater chemical composition of clays. Main uncertainties are related to kinetic calcite dissolution and variations in CO<sub>2</sub>(g) pressure.

### C.2.3 THC modelling of the permeation test

A THC numerical model of a long-term permeation test performed on a 2.5 cm long sample of saturated FEBEX bentonite (Fernández et al. 2002) was performed during the FEBEX II project (Samper et al. 2005b, Enresa 2006a, 2006d). In this test, porewater solution of the saturated bentonite sample was flushed with granitic water. Water flux and chemical composition of effluent waters were monitored during almost 4 years. The initial water content and the dry density of the FEBEX compacted bentonite were, respectively, 23.1 % and 1.65 Mg/m<sup>3</sup>.

This long-term permeation test was interpreted numerically using single and double porosity models and three conceptual geochemical models. THC model results lead to the following conclusions:

- There are uncertainties on the appropriate flow boundary conditions for the permeability test. Although a constant pressure (Dirichlet) boundary condition seems more appropriate to represent the injection pressure, the fact that the flow rate decreased during the experiment makes us believe that a specified flux (Neumann) boundary condition represents better the flow through the bentonite samples. However, the Neumann condition leads to solute fluxes which exceed measured fluxes. A numerical model with unsaturated flow should be constructed in order to test this hypothesis.
- A single porosity model leads to results which match the overall trends of measured breakthrough curves for most species. In general, measured data fall within the bands of computed breakthrough curves with conceptual models CGM-0, CGM-1 and CGM-2. The largest differences among models are found for sulphate, bicarbonate and calcium.
- The single porosity model fails to reproduce the early part of the breakthrough curve of chloride. The fit of this curve improves noticeably when anion exclusion is considered. Models without exclusion fail to reproduce the breakthrough curve of chloride. Our results indicate that chloride can access 35 % of the mobile porosity and 58 % of the immobile pore space.
- Chloride and sodium data tend to firmly support the double porosity model. The relevance of double porosity for other species remains to be ascertained.

- Single and double porosity models fail to reproduce the bicarbonate breakthrough curve, possibly because the model does not account for possible changes in  $\text{CO}_2(\text{g})$  pressures. The results for bicarbonate improve when a double porosity is used.

Samper et al. (2008a) present an updated inverse single- and dual-continuum multicomponent reactive transport model of this long-term permeation. The model accounts for solute advection and diffusion and geochemical reactions such as aqueous complexation, acid-base, cation exchange, protonation/deprotonation by surface complexation and dissolution/precipitation of calcite, chalcedony and gypsum. Local equilibrium is assumed for all these processes. Given the difficulties of deriving reliable data on bentonite porewater chemistry, they adopted as prior estimate of initial composition of bentonite porewater that derived by Samper et al. (2005a) from a squeezing experiment (CGM-0) at 23.8 % water content because it is based on experimental conditions close to those of the permeation test.

As in previous studies of bentonite porewater chemistry on batch systems, which attest the relevance of protonation/deprotonation on buffering pH, the results confirm that protonation/deprotonation is a key process in maintaining a stable pH under dynamic transport conditions. Breakthrough curves of reactive species are more sensitive to initial porewater concentration than to effective diffusion coefficient. Optimum estimates of initial porewater chemistry of saturated compacted FEBEX bentonite are obtained by solving the inverse problem of multicomponent reactive transport. While the single-continuum model (SCM) reproduces the trends of measured data for most chemical species, it fails to match properly the long tails of most breakthrough curves. The dual-continuum reactive transport model (DCM) is able to match these tails (see Fig. C-1).

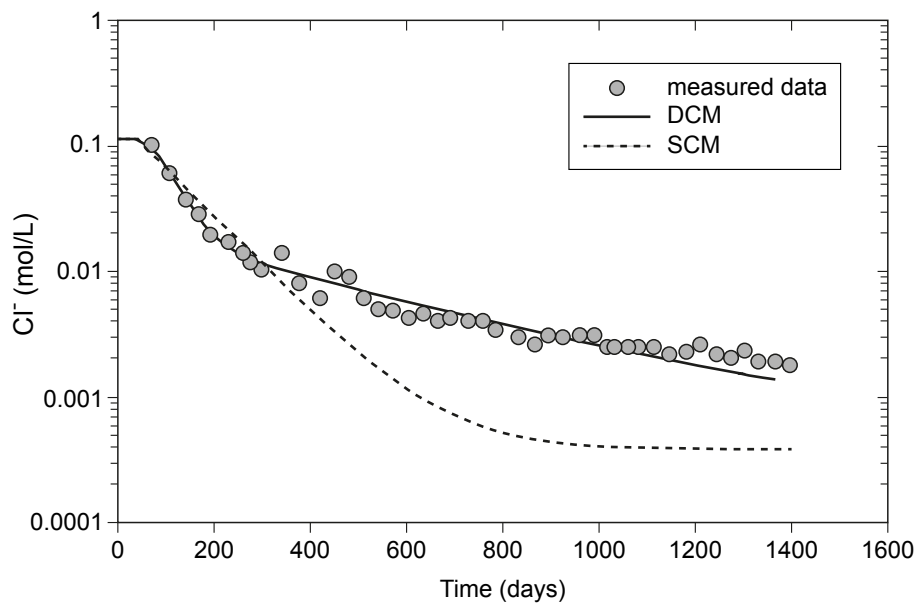


Fig. C-1: Measured and computed breakthrough curves of chloride with SCM and DCM (Samper et al. 2008b).

### C.2.4 THC/THmC modelling of the CT23 test

A series of laboratory tests were performed within the FEBEX project to study water flow and reactive solute transport in compacted bentonite during simultaneous heating and hydration. One of such tests was performed on the cell CT23 (Huertas et al. 2000). A 4.29 kg FEBEX bentonite block with 13 cm in height and 15 cm of diameter was placed in a stainless steel cylindrical hermetic cell. A heater maintained a constant temperature of 87.5 °C in the upper part of the cell. At the same time, the lower part of the bentonite block was hydrated with distilled water injected at a pressure of 1 MPa through a 2.4 cm thick porous stone. The initial dry density of the bentonite is 1.65 Mg/m<sup>3</sup>. After 183 days of heating and hydration the heater was switched off, hydration was stopped and the bentonite sample was allowed to reach the ambient temperature. The bentonite sample took 486 cm<sup>3</sup> of water and its gravimetric water content increased from 13.3 % at t = 0 (initial saturation degree of 56.4 %) to an average water content of 26.1 % (saturation degree of 94 %).

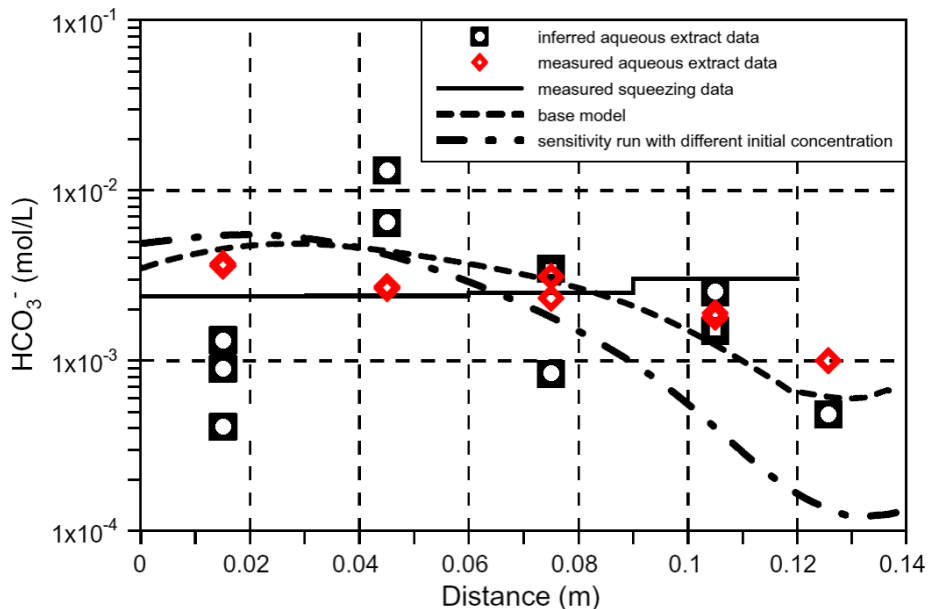


Fig. C-2: Comparison of computed  $\text{HCO}_3^-$  concentrations and inferred AET at the end of the CT23 test ( $t = 183$  days).

Also shown are measured squeezing and AET data as well as the results of a sensitivity run with a different initial concentration (Zheng et al. 2010).

Zheng et al. (2010), following the previous THC model of the CT23 test developed during the FEBEX II project (Samper et al. 2005b, Enresa 2006a, 2006d), present a non-isothermal multi-phase flow and multicomponent reactive solute transport model (THmC model) for a deformable medium of the CT23 test performed by CIEMAT on a sample of compacted FEBEX bentonite. Besides standard solute transport and geochemical processes, the model accounts for solute cross diffusion and thermal and chemical osmosis. Bentonite swelling is solved with a state-surface approach. The THM model is calibrated with transient temperature, water content and porosity data measured at the end of the experiment. The reactive transport model is calibrated with porewater chemical data derived from aqueous extract data. Model results confirm that thermal osmosis is relevant for the hydration of FEBEX bentonite, while chemical osmosis can be safely neglected. Dilution and evaporation are the main processes controlling the concentration of conservative species. Dissolved cations are mostly affected by calcite

dissolution/precipitation and cation exchange reactions. Dissolved sulphate is controlled by gypsum/anhydrite dissolution/precipitation. pH is mostly buffered by protonation/deprotonation via surface complexation. Computed concentrations agree well with inferred aqueous extract data at all sections except near the hydration boundary where cation data are affected by a sampling artefact. The fit of Cl<sup>-</sup> data is excellent except for the data near the heater. The largest deviations of the model from inferred aqueous extract data occur for dissolved SO<sub>4</sub><sup>2-</sup>, which is underpredicted by the model. There are uncertainties on the amount of gypsum available for dissolution and its dissolution mechanism (kinetics or local equilibrium).

### C.3 THC/THmC modelling of the Mock-up Test

UDC has developed THC and THmC models of the FEBEX Mock-up Test in order to predict the transport patterns of artificial tracers (iodide) and predict the THC/THmC performance of the engineered barrier of the Mock-up Test (Enresa 2000, Samper et al. 2005b, Enresa 2006a, 2006d). Some of the tasks performed by UDC within the FEBEX I and FEBEX II projects were the following:

- Develop a 3D TH model with axial symmetry.
- Analyse discrepancies between model predictions and measured data. Possible plausible explanations to the observed discrepancies are the change of intrinsic permeability with ionic strength and the effect of chemical and thermal osmosis.
- Modelling the overheating episode. Model results indicate that the overheating affected hydrodynamic conditions although only slightly due to its short duration. The model captures the trends of measured temperature although it cannot reproduce the sharp temperature profile. The model captures the trend of measured relative humidity. In the middle part of the barrier, however, it fails to reproduce the slow recovery phase after overheating.
- Update predictions of the migration of iodide using the revised TH model, in which molecular diffusion coefficient and accessible porosity are those estimated by the inverse model for iodide migration for the In Situ Test.
- Calibration of the TH model using thermal and hydrodynamic data collected during FEBEX II.
- Update predictions of the THC evolution of the barrier. Compared with the predictions of FEBEX I (Enresa 2000), chloride concentrations near the heater are larger when the variable permeability function is used because less water enters into the bentonite barrier and consequently the water content near the heater is lower. At 30 years, the chloride pattern is flat. For the same reason, the time needed to reach steady state is larger than the prediction of FEBEX I. In the previous model, steady state concentrations were achieved in 10 years (Enresa 2000). In the updated model, steady concentrations are attained after 20 years. The trends of most of the chemical species, except for bicarbonate, show similar patterns to those of chloride, even though these species are subject to calcite and anhydrite mineral dissolution/precipitation and cation exchange. Changes in the composition of the bentonite exchange complex are larger near the heater than in the hydration boundary.

Zheng & Samper (2008) present the most recent THmC model of the FEBEX Mock-up Test. This 1D axisymmetric coupled THmC model of the FEBEX Mock-up Test, which accounts for thermal and chemical osmosis and bentonite swelling with a state-surface approach, reproduces measured temperature and cumulative water inflow data. It fits also relative humidity data at the outer part of the buffer but underestimates relative humidity near the heater. Dilution due to hydration and evaporation near the heater are the main processes controlling the concentration

of conservative species of the FEBEX Mock-up Test, while proton surface complexation, mineral dissolution/precipitation and cation exchange affect significantly reactive species as well. Results of sensitivity analyses to chemical processes show that pH (see Fig. C-3) is mostly controlled by proton surface complexation, while dissolved cations concentrations are controlled by cation exchange reactions.

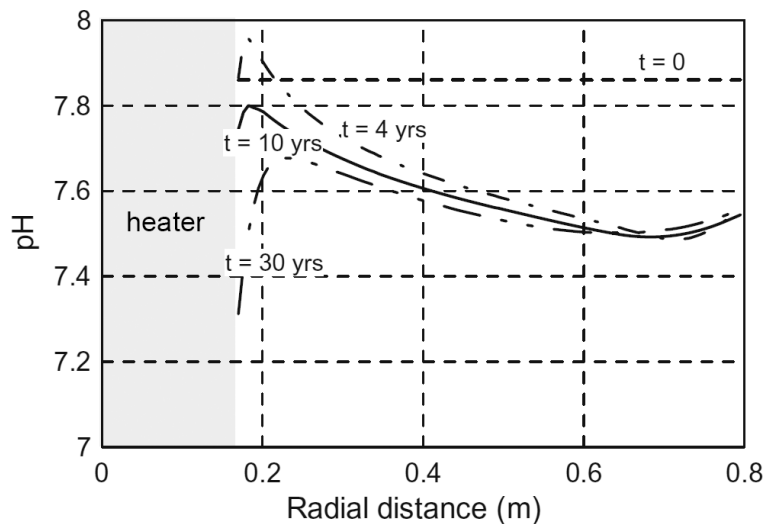


Fig. C-3: Spatial distribution of computed pH at different times in the Mock-up Test (Zheng & Samper 2008).

#### C.4 THC/THmC modelling of the In Situ Test

UDC has developed THC and THmC models of the FEBEX In Situ Test in order to predict the transport patterns of added artificial tracers (iodide and deuterium), predict the THC/THmC performance of the engineered barrier of the In Situ Test and test the THC/THmC predictions with dismantling data of Heater # 1 of the In Situ Test (Enresa 2000, Samper et al. 2005b, Enresa 2006a, 2006d). The THC model of the In Situ Test has been revised and updated by incorporating the conclusions drawn from the THC model of the Mock-up Test. The following tasks have been performed within the FEBEX I and FEBEX II projects:

- Analyse the discrepancies between model predictions and measurements.
- Review and update THC predictions by correcting numerical problems.
- Perform sensitivity analyses to molecular diffusion, dispersivities, and chemical composition of granite porewaters.
- Update model predictions of tracer migration for deuterium and iodide. Available deuterium data do not allow drawing clear conclusions due to: (1) Although precision of deuterium data of aqueous extract samples is 0.8 ‰, this analytical error translates into, and (2) uncertainties on glass ampoules breaking. Only 3 were found broken. Most likely glass ampoules broke during the test, because if they had broken during dismantling, clay samples near the glass should still show high deuterium ratios. However, since the amount of deuterated water added was not large enough, there is not clear evidence of deuterium migration.
- Update and compare THC predictions to AET data from cold and hot sections of Heater # 1.

The THC model results of the FEBEX In Situ Test was tested with data collected after the dismantling of Heater # 1. Geochemical data of the In Situ Test were obtained from aqueous extract tests performed at low solid-to-liquid ratios. The interpretation of these data requires the use of hydrogeochemical models to account for the geochemical reactions that occur in the bentonite samples during the aqueous extraction tests (Zheng et al. 2008).

Re-interpreted data were compared to THC model predictions of the In Situ Test performed with three possible conceptual geochemical models. The comparison of predicted and inferred values using data from Sections 19 and 29 (hot areas) and 12 (cold area) indicates that:

- THC predictions capture the general trends of most chemical species in hot and cold areas except for sulphate and bicarbonate.
- Concentrations of most chemical species are larger near the heater due to bentonite pore-water evaporation than in the granite-bentonite interphase due to water hydration.
- The spatial distribution of chemical species is affected by the inwards displacement of the hydration front, evaporation, diffusion processes, mineral dissolution/precipitation and cation exchange.
- Although the model tends to over-predict chloride concentrations near the granite-bentonite interphase at Section 29, inferred aqueous extract and squeezing data at Section 19 fall closer to the band of computed values with models CGM-0, CGM-1 and CGM-2. In Section 12, the behaviour is the same near the granite-bentonite interphase but squeezing data for the sample BB 12-10 fall closer to the inferred aqueous extract data.
- Dissolved cations ( $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ) show similar trends to those of chloride. Even though these species are subject to chemical reactions (mineral dissolution/precipitation and cation exchange), these processes are not sufficiently strong compared to dilution and evaporation processes to change their concentration patterns.
- Models CGM-1 and CGM-0 seem to fit calcium inferred aqueous extract data better than model CGM-2 near the heater in the hot section (Section 29). THC predictions of calcium in the cold section (Section 12) with model CGM-0 do not fit inferred aqueous extract data, but those with CGM-1 and CGM-2 reproduce the trend of measured data. Such a discrepancy could be related to the role of anhydrite. Near the granite-bentonite interphase squeezing data fall closer to the band of computed and re-calculated values with the three models in both sections.
- Computed results of magnesium, sodium and potassium with models CGM-0, CGM-1 and CGM-2 reproduce the general trends of inferred aqueous extract data in both sections. Squeezing values for potassium are smaller than expected.
- The trend of computed sulphate concentrations of bentonite porewater is controlled by the dilution effect of granitic water, water evaporation and anhydrite dissolution/precipitation. Sulphate inferred aqueous extract data are greater than computed values. Model predictions are more coherent with squeezing data than to inferred aqueous extract data.

Samper et al. (2008a) present a THC model of the In Situ Test up to dismantling, utilising a common thermo-hydraulic model and three different geochemical conceptual models for the bentonite porewater. The model achieves a good match to temperature in the buffer and the general trend of water content. However, the overall shape of the water content is not matched as the model assumes a constant heater boundary condition and does not account for swelling and hence the observed gradient in dry density (Villar et al. 2005). The models reproduce the general trend of  $\text{Cl}^-$  and cations which follow the same trend (can be considered as acting as a

conservative tracer). The model systematically underestimated  $\text{SO}_4^{2-}$  concentrations which may be related to gypsum/anhydrite dissolution. The pattern of  $\text{HCO}_3^-$  concentration data is not fitted well by any of the models which may relate to  $\text{CO}_2$  degassing.

Following on from work within FEBEX I & II, further THMC modelling of FEBEX-related tests have included models of:

- Mock-up Test: Zheng & Samper (2008)
- laboratory heating/hydration tests: Zheng et al. (2010)
- In Situ Test: Zheng et al. (2011)

Zheng et al. (2011) present the most recent THMC modelling of the FEBEX In Situ Test. The model is a development of previous work by Samper et al. (2008a). Samper et al. (2008a) report significant discrepancies between calculated and measured concentrations for most chemical species. The revised model includes thermal osmosis and bentonite swelling to address this problem and builds on the model developed for the Mock-up (Zheng & Samper 2008). Sensitivity analyses are used to understand the influence of different assumptions (e.g. Fig. C-4). The model demonstrates the influence of intrinsic permeability, bentonite swelling and thermal osmotic permeability on the porewater chemistry. Inclusion of a state-surface bentonite swelling model together with thermal osmosis allows a reasonable match to the  $\text{Cl}^-$  and cations which largely follow the  $\text{Cl}^-$  trend ( $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ). The models show very little influence of chemical osmosis. Zheng et al. (2011) also demonstrate the importance of calcite dissolution, cation exchange reactions and gypsum/anhydrite dissolution/precipitation on the geochemical evolution of the buffer.

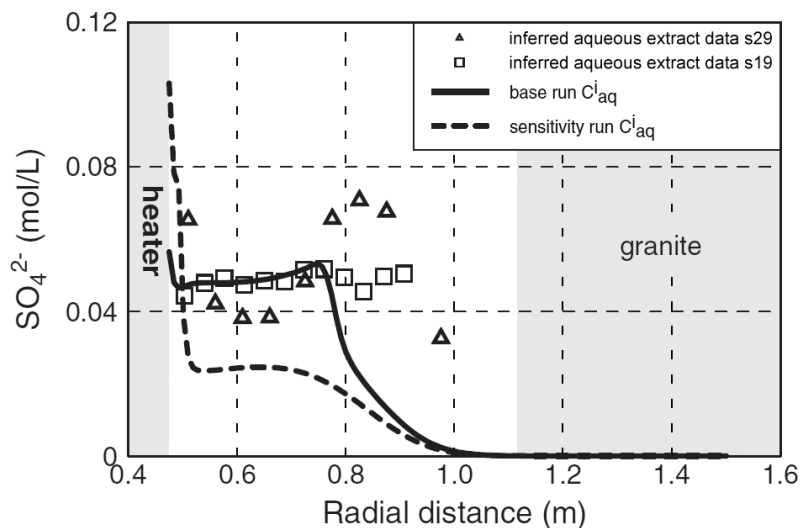


Fig. C-4: Computed (lines) and inferred  $\text{SO}_4^{2-}$  concentrations at Sections 19 and 29 (symbols) after 1'930 days in the In Situ Test.

Computed concentrations are shown for two initial concentrations derived by AET and squeezing (Zheng et al. 2011).

Model results deviate from measurements at the interfaces, i.e. close to the heater or the rock. The authors suggest this may be due to several processes such as  $\text{CO}_2$  degassing, bentonite volume changes or vapour transport to the rock or a combination of those.  $\text{HCO}_3^-$  and pH data

cannot be explained by the model. Zheng et al. (2011) suggest this may be due to CO<sub>2</sub> degassing and transport within the buffer. Significant uncertainties associated with the models therefore remain and include:

- magnitude of thermal osmotic permeability
- accessibility of water within the different porosities in the bentonite
- quantity of gypsum in the bentonite available for dissolution and dissolution mechanism
- initial bentonite porewater composition (see Fernández et al. 2004, Fernández & Rivas 2005, Zheng et al. 2008)
- Assumption of a closed (airtight) system

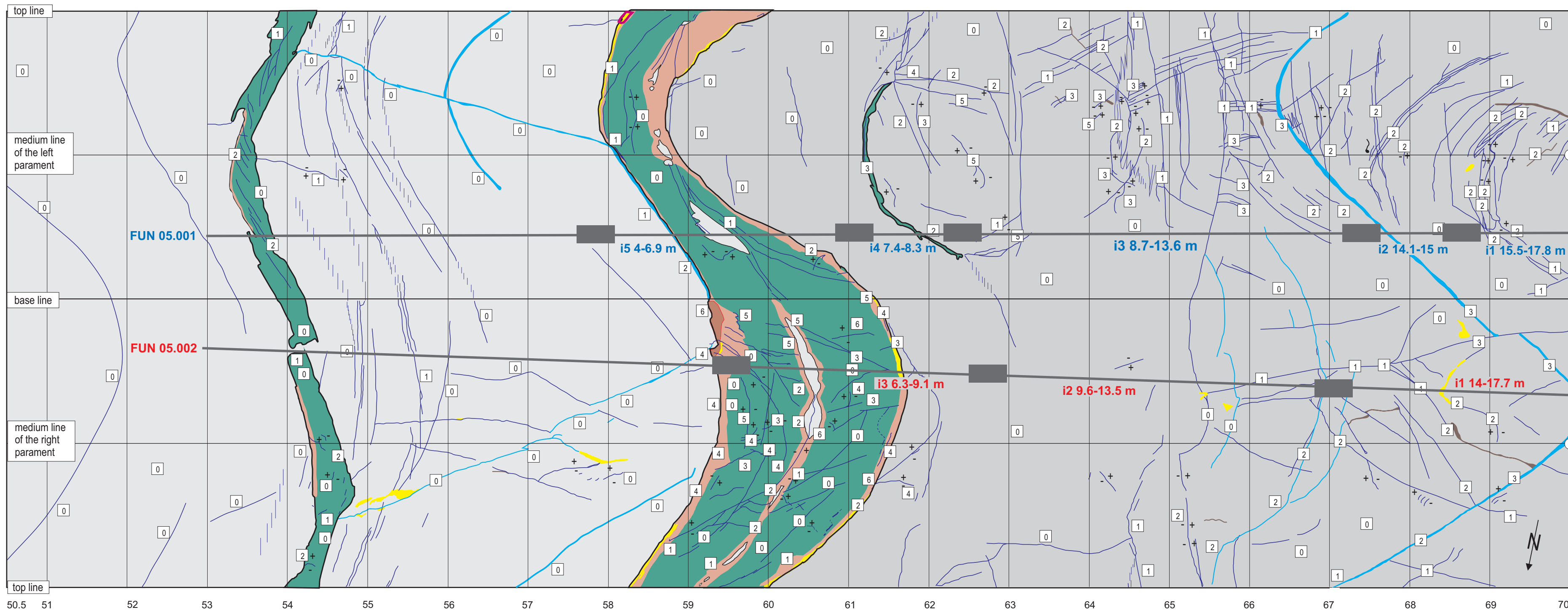
## C.5 Summary and conclusions

A significant improvement in THC/THmC modelling of the clay barrier has been achieved during the FEBEX project. Available THC codes at the beginning of the project could handle only non-isothermal multiphase flow and transport with no geochemical processes or isothermal saturated flow and reactive transport. Novel numerical methodologies and sophisticated THC/THmC codes were developed during the course of the project which could handle in a general manner the observed thermo-hydro-geochemical couplings and account for the most relevant features of the THC conceptual model. Such codes are at the cutting-edge of coupled THC/THmC models for porous media. THC/THmC models were constructed by using such codes and relying on: 1) data provided by a wide range of small-scale laboratory tests, 2) thermal and hydrodynamic data from the Mock-up Test, and 3) thermal, hydrodynamic and geochemical data from partial dismantling of the In Situ Test during the summer of 2002. The ability of THC models to reproduce most of the observed THC patterns under such a large number of conditions enhances confidence in their predictive capabilities.






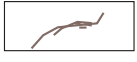
The most recent developments in THC/THmC models have addressed the multiple-porosity behaviour of bentonite and the mechanical-geochemical couplings within the context of the PEBS European Project (2010 – 2014). UDC extended the capabilities of THC/THmC codes to deal with mechanical and geochemical couplings (thus leading to fully coupled THMC models), account for porosity changes caused by swelling phenomena, and consider reactive gases (i.e. CO<sub>2</sub> degassing) (Samper et al. 2014a). Some of these developments were tested with data from the FEBEX Mock-up Test.

Most of the THC/THmC analysis effort has been devoted to constructing thermo-hydro-geochemical models for the main geochemical processes controlling the geochemical evolution of the clay barrier in terms of major ion composition, pH, and alkalinity. There are some processes which are relevant for performance assessment, such as redox reactions and interactions of corrosion products, but were not addressed within the FEBEX project. Within the PEBS project, existing THmC models have been applied to the modelling of the interactions of corrosion products and bentonite, and the interactions of concrete and bentonite (Samper et al. 2014b).



Improved conceptual geochemical models have been developed within the PEBS project in which a distinction is made between intra-aggregate and inter-aggregate water for the purpose of hydrogeochemical modelling. Dual porosity models using the dual continuum model (DCM) approach have been developed. Such models should be tested in the future with additional thermo-hydro-geochemical data such as the data from the dismantling of the second heater of the FEBEX In Situ Test.



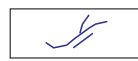

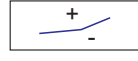

**Lithology:**

-  CAGr (Central Aare Granite)
-  CAGr light
-  Lamprophyre
-  Xenolith or basic inclusions
-  Quartz - feldspar (-biotite) inclusions
-  Biotite accumulations

**Disturbed zones:**

-  Disturbed zone
-  Breakout

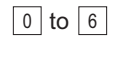
**Structures:**

-  Fractures with fillings of biotite, muscovite, chlorite and epidote (calcite in lamprophyre)
-  En echelon fractures
-  Steps
-  Veins filled with quartz, feldspar, biotite, muscovite, epidote or calcite

**Boreholes:**

-  **i5 4-6.9 m** FUN 05.001 interval number and position
-  **i3 6.3-9.1 m** FUN 05.002 interval number and position

**Hydrogeology:**

-  Water inflow zones (qualitative):
- in matrix [m<sup>2</sup>]:
- Range 0: Q ~ 17e-3 ml/min/m<sup>2</sup>
- Range 1: Q ~ 42e-3 ml/min/m<sup>2</sup>
- in fractures [m]:
- Range 2: Q ~ 20e-3 ml/min/m
- Range 3: Q ~ 37e-3 ml/min/m
- Range 4: Q ~ 70e-3 ml/min/m
- in points:
- Range 5,6: Point inflow

Water inflow values were measured at points in the FEBEX tunnel using cellulose sheets

Azimuth of Febex tunnel (from 0 to 70 m): 258.3°

**Coordinates of measurement-points:**

-  <sup>1</sup> 667423.617 159327.271 1730.21
-  <sup>2</sup> 667423.180 159329.490 1730.20

Mapping: Felip Ortuño Gobern, Ciemat, Spain  
 Julio Pardillo, Ciemat, Spain  
 Hannes Dollinger, Geotechnical Institut AG, Switzerland

Drawing: Andreas Möri, Geotest, Switzerland

<b>nagra</b>	<b>NTB 15-04</b>
Hydrogeological map of the FEBEX tunnel from 50.5 m to 70 m	
DAT.: March 2016	<b>Map 1</b>