



EUROPEAN
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European
Research Area



Long-term
Performance of
Engineered
Barrier
Systems

Long-term Performance of Engineered Barrier Systems

PEBS

DELIVERABLE (D-N°:D5-5)

Documents of 1st Workshop

Contract (grant agreement) number: **FP7 249681**

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Date of issue of this report: 06/06/12

Start date of project : **01/03/10**

Duration : **48** Months

| | | |
|--|---|----|
| Project co-funded by the European Commission under the Seventh Euratom Framework Programme for Nuclear Research & Training Activities (2007-2011) | | |
| Dissemination Level | | |
| PU | Public | PU |
| RE | Restricted to a group specified by the partners of the PEBS project | |
| CO | Confidential, only for partners of the PEBS project | |

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| Christophe Davies | 1 digital file | no paper copy |

(D-N°: [D5-5](#)) – Documents of 1st Workshop

Dissemination level : [PU](#)

Date of issue of this report : [06/06/12](#)

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1. Summary

This workshop is part of a project, that carries out cutting edge research for the engineering and the construction and operations of a underground waste disposal site for heat generating waste. The project has also to be understood as a kind of action that follows the former project NF-PRO. PEBS takes some of the results and recommendations from NF-PRO for aimed work for further and more detailed surveys. Most of the partners are well known from the NF-PRO.

The European Commission encouraged to install two workshops exclusively for the regulatory authorities to discuss open and without comment from other parties technical, mineralogical, geotechnical, mathematical and mining concepts for barriers for future European repositories which are engineered to resist all relevant szenarios

In a first workshop the relevant szenarios and an analysis of system evolution during early post-closure period, the Impact on long-term safety functions and an analysis of impact on long term safety will be presented and discussed. The team will present background and first results of various underground and laboratory tests.

In the second workshop, proposed for the end of the project (about December 2013 or January 2014) the results of Work Package 4, which includes the Analysis of impact on long-term safety and guidance for repository design and construction will be compared and discussed in relation to the szenarios from Work Package 1.

The PEBS project includes 7 work packages. Work packages 1 to 4 and the Chinese work package B are concentrating on research and technical work of RTD type. The work packages 5 and 6 focus on dissemination of results and the management of the Project. The workshop was installed as part of the Work Package 5 Dissemination.

2. Objective of the workshop

The objectives of the workshop are:

The workshop will be arranged as a closed shop workshop to present and discuss the results of Work Package 1 only to experts of European/abroad Regulatory Authorities. This workshop will follow such objectives as

- Discussion and analysis of Identified important processes (FEPs) during the early evolution of the EBS
- Discussion of the results of the current treatment of the early evolution of the EBS in long-term safety assessments for spent nuclear fuel
- Discuss how the short-term transients will/may affect the long-term performance and the safety functions of the repository.
- Discussion of merits and shortcomings of the current treatment
- Discussion of future assessments related to events in the early evolution of the EBS.

It is especially intended, to estimate all constructive comments on the singular content and the objectives of the PEBS project also under the aspect to review parts of the work program.

3. Content and Agenda of the Workshop

The agenda:

First half day:

- Swisstopo Presentation, Mont Terri Project (Annex 1, Title: Mont Terri Project)
- Field trip to the Mont Terri Underground Research Laboratory

Second day:

- PEBS General Overview, Objectives, Management (Annex 2, Title: PEBS General Overview, Objectives, Management)
- Overview and current results of work package 1 (Analysis of system evolution during early post-closure period, Impact on long-term safety functions) and work package 4 (Analysis of impact on long term safety), (Annex 3, Title: Overview and current results of work package 1 (Analysis of system evolution during early post-closure period, Impact on long-term safety functions) and work package 4 (Analysis of impact on long term safety))
- Overview of work package 2 (Experimentation on key EBS processes and parameters), (Annex 4, Title: Experimentation on key EBS processes and parameters)
- THM and THM-C laboratory experiments (Annex 5, Title: THM and THM-C laboratory experiments)
- HE-E experiment (THM field experiments), (Annex 6, Title: HE-E experiment in the VE Test Section, EBS behavior immediately after repository closure in a clay host rock)
- Overview of WP3 (Modelling of short-term effects and extrapolation to long-term evolution), (Annex 7, Title: Overview of Modelling Tasks (WP3))
- Coupled thermal-hydraulic-chemical modelling taking into account (certain) mechanical effects (Annex 8, Title: Coupled thermal-hydraulic-chemical modeling taking into account some mechanical effects)
- Coupled thermal-hydraulic-mechanical modeling of the bentonite buffer (Annex 9, Title: Coupled thermo-hydro-mechanical modeling of the bentonite buffer)

4. Organisation of the workshop

The overall organization includes scheduling, decision of the content, allocation of speakers and determination of venue. The PEBS team was very pleased, that swisstopo as the leading organization of the Mont Terri Project arranged the use of the INFORMATION CENTER for this workshop without charge.

5. Further Steps

Again exclusively for Regulatory Authorities a 2nd workshop will be arranged together with the final workshop at the end of the project (December 2013 or January 2014). It will be prepared as a closed shop workshop only for experts from Regulatory Authorities. Results and draft concepts will be presented. Impacts on licensing will be discussed.

This workshop will be in line with the results of the WP 4 and will reflect also the objectives of the 1st Workshop with such objectives as:

- Discussion the findings i) of the WP2 and WP3 experiments and models, ii) of development of a more complete qualitative process-related description of the early evolution phase of the repository (the first several hundred years) and the residual uncertainties in the evolution, iii) of possible different behaviours of the system that may be implied by the uncertainties or disagreement between models and experiments
- Presentation and discussion of the results of experiments and models and their significance in relation to long-term safety functions of the buffer, canister and host rock (clay and crystalline) in a quantitative fashion, including the importance of residual uncertainties (i)importance of the transient period with regard to the long-term characteristics particularly relevant to system performance and long-term safety; ii) of uncertainties arising from disagreement between models and experiments and their implications for extrapolation of results, with particular emphasis on possible impacts on safety functions.
- Presentation of an improved and more complete approach to integrating the thermal and resaturation phase of the repository with the long-term steady state phase of repository evolution.

6. Annexes

| | |
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| Annex 2, PEBS General Overview, Objectives, Management | Page 18 |
| Annex 3, Overview and current results of work package 1 (Analysis of system evolution during early post-closure period, Impact on long-term safety functions) and work package 4 (Analysis of impact on long term safety) | Page 30 |
| Annex 4, Experimentation on key EBS processes and parameters | Page 43 |
| Annex 5, THM and THM-C laboratory experiments | Page 55 |
| Annex 6, HE-E experiment in the VE Test Section, EBS behavior immediately after repository closure in a clay host rock | Page 82 |
| Annex 7, Overview of modelling Tasks (WP3) | Page 98 |
| Annex 8, Coupled thermal-hydraulic-chemical modelling taking into account some mechanical effects | Page 114 |
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Mont Terri Project



Visit of Mont Terri rock laboratory

Participants of PEBS Workshop



25 April 2012



www.mont-terri.ch

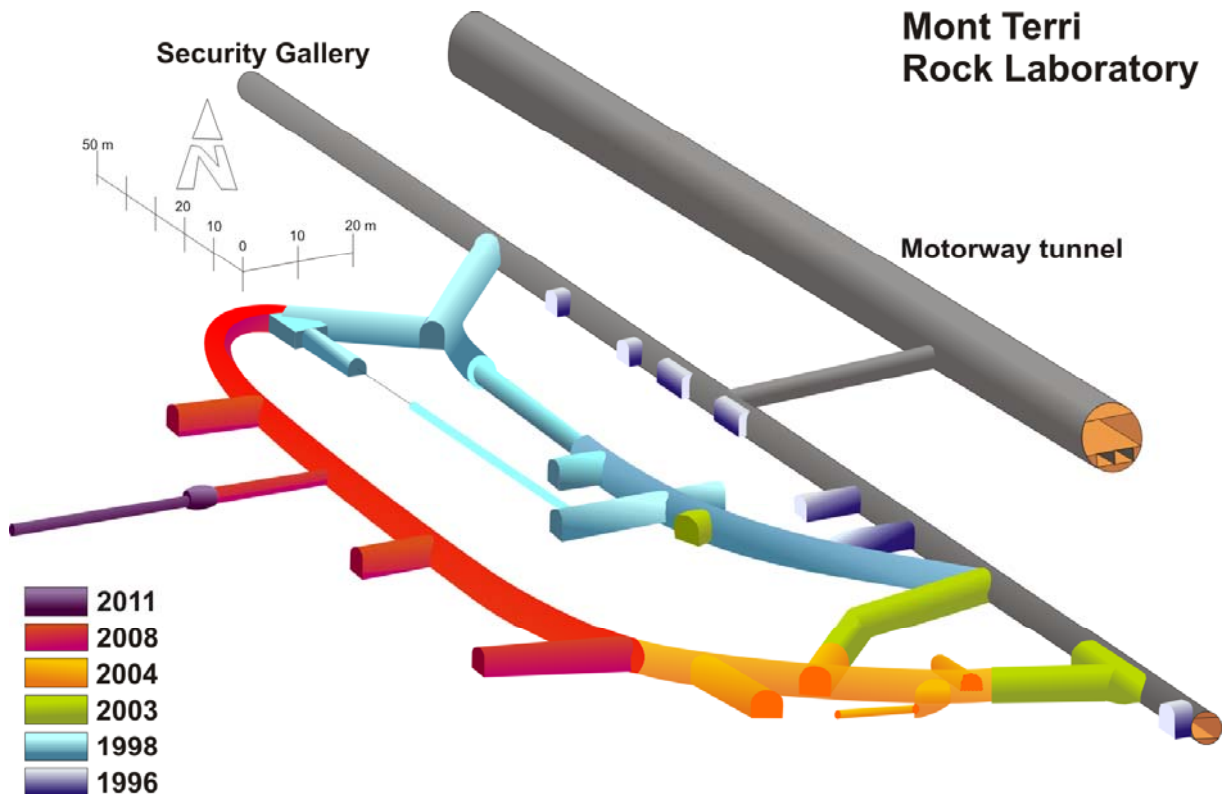
Paul Bossart



Security Gallery

Mont Terri
Rock Laboratory

Motorway tunnel





The Partners



Mont Terri Project



swisstopo
nagra
ENSI

swisstopo Bundesamt für Landestopografie
NAGRA Nationale Genossenschaft für die Lagerung von radioaktivem Abfall
ENSI Eidgenössisches Nuklearsicherheitsinspektorat



ANDRA Agence Nationale pour la Gestion des Déchets Radioactifs
IRSN Institut de Protection et de Sûreté Nucléaire



BGR Bundesanstalt für Geowissenschaften und Rohstoffe
GRS Gesellschaft für Reaktorsicherheit und Strahlenschutz



ENRESA Empresa Nacional de Residuos Radiactivos, S.A.



SCK•CEN Studiecentrum voor Kernenergie, Mol



JAEA Japan Nuclear Cycle Development Institute



OBAYASHI Obayashi Corporation



CRIEPI Central Research Institute of Electric Power Industry



NWMO Nuclear Waste Management Organisation, Toronto



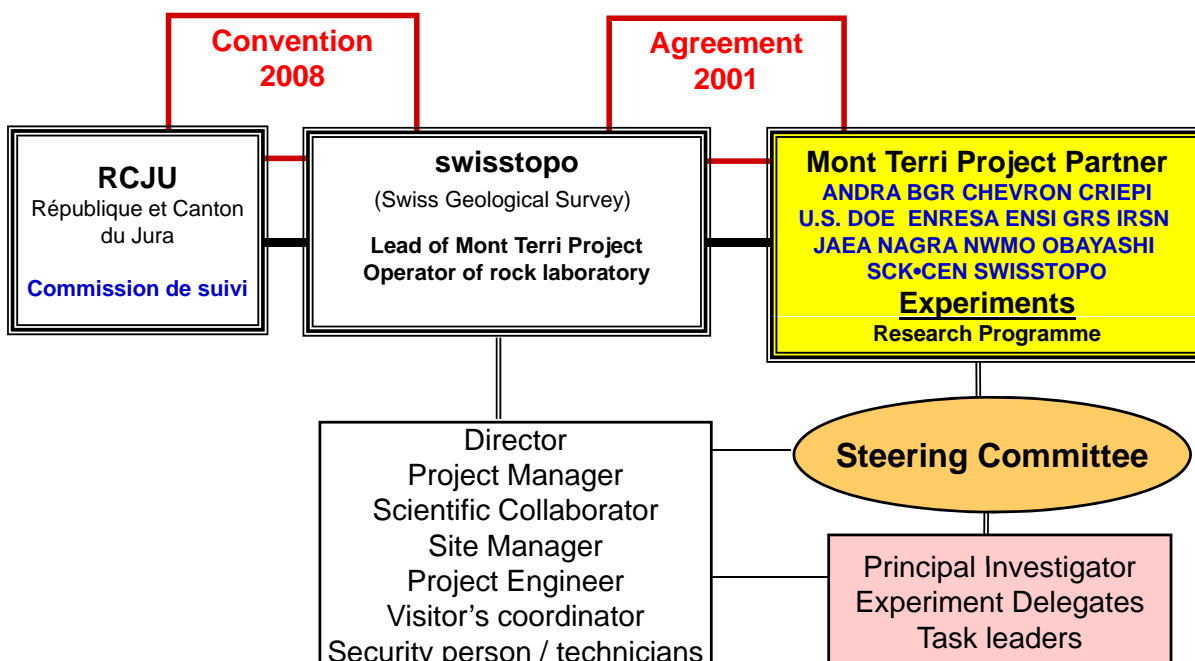
U.S. DOE Department of Energy, Washington DC
Chevron Chevron Energy Technology Company, Houston



Organisation

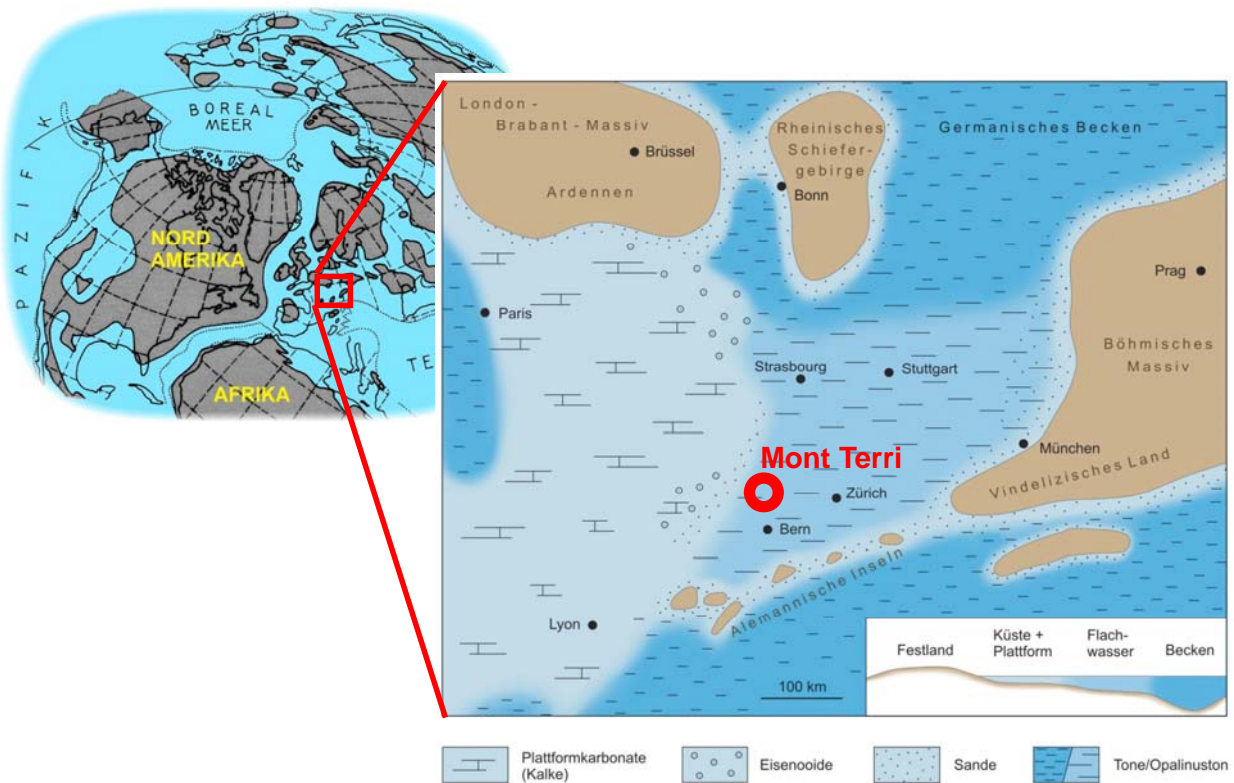
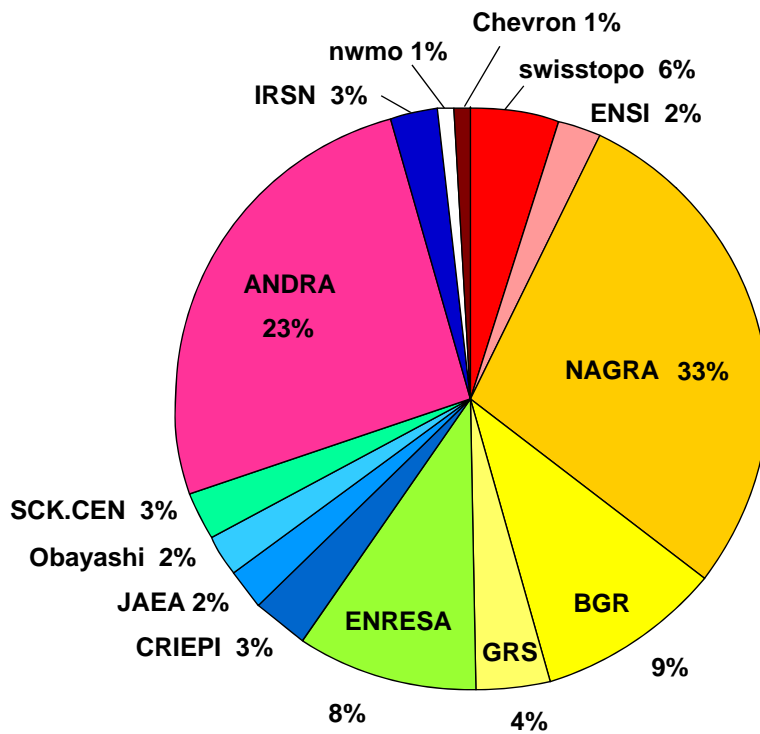


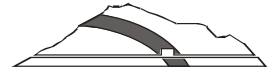
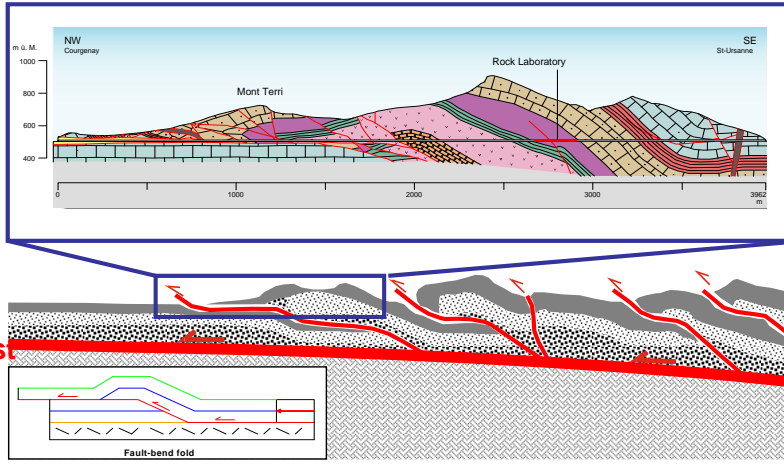
Mont Terri Project





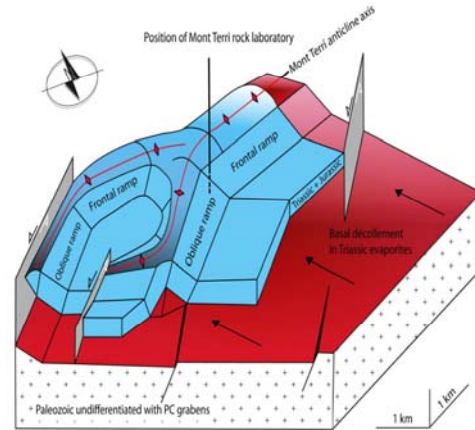
1996 – Mitte 2012: 63.4 Mio CHF



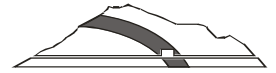


Mont Terri Project

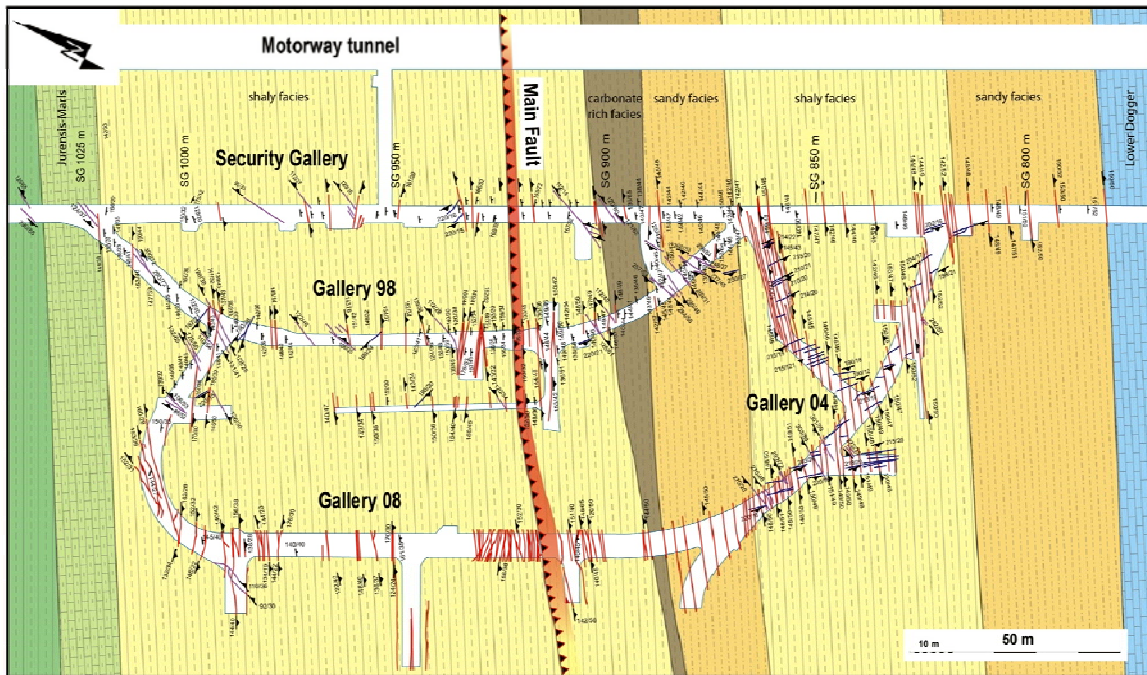
<http://www.mont-terri.ch/internet/mont-terri/de/home/geology.html>



Geological map of the Mont Terri rock laboratory



Mont Terri Project



Stratigraphy:

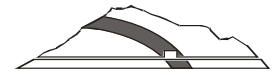
- "Lower Dogger" limestones (Dogger, Bejocian)
- Sandy facies
- Carbonate-rich sandy facies
- Shaly facies
- Jura's Marls (Elias upp. Toarcian)
- Opalinus Clay
- Posidonia shales (Elias. low. Toarcian)

Fault systems:

- dipping fault system (bedding parallel)
- SW to S dipping fault system
- N and NNE trending fault systems
- SSE dipping thrust zone (Main Fault)



“Key-Parameters”



Mont Terri Project

PARAMETRES

RANGE

BEST ESTIMATE

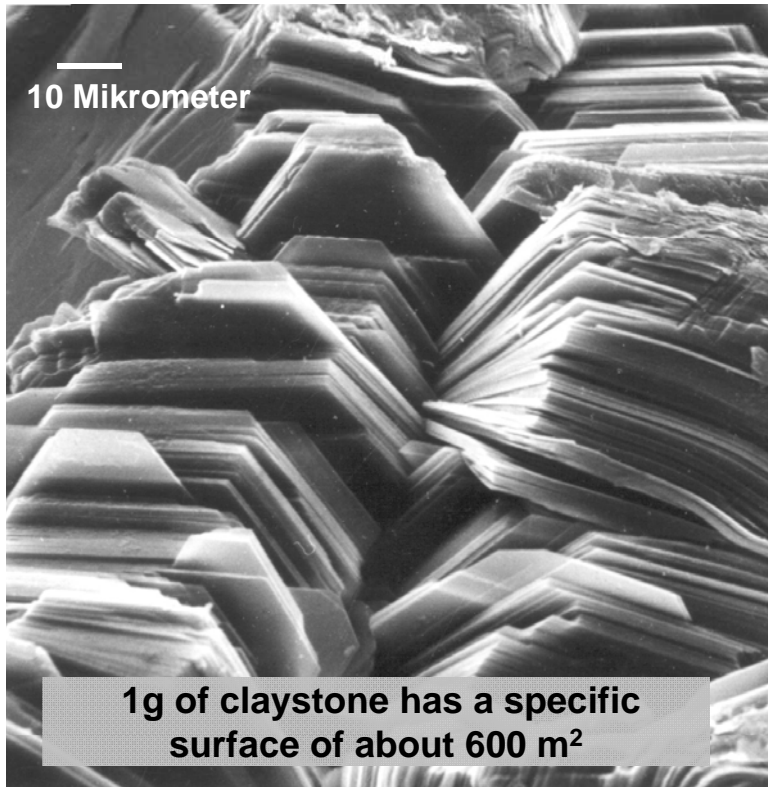
| | | |
|--|----------------|-------|
| Bulk density, sat. (g cm ⁻³) | 2.40 – 2.53 | 2.45 |
| Water content (wt%) | 5.5 – 8.9 | 6.6 |
| Total (physical) porosity (vol%) | 14 – 25 | 18 |
| Water loss porosity at 105°C (vol-%) | 13 – 21 | 16 |
| Effective porosity for chloride (vol%) | 8 – 10 | 9 |
| Hydraulic conductivity (ms ⁻¹) | *2E-14 – 1E-12 | 2E-13 |
| Thermal Conductivity (Wm ⁻¹ K ⁻¹) | *1.0 – 3.1 | 1.7 |
| Heat capacity (J Kg ⁻¹ K ⁻¹) | 750 – 1000 | 860 |
| Total dissolved solids in pore water (g/l) | 5 - 20 | 12 |
| Uniaxial compressive strength (MPa) | *4 – 28 | 11 |
| Young’s modulus (MPa) | *6000 – 12000 | 9000 |
| Poisson’s ratio (-) | *0.16 – 0.38 | 0.25 |
| Shear modulus (MPa) | *800 – 1600 | 1200 |

* Values are dependant on bedding anisotropy



Mont Terri Project

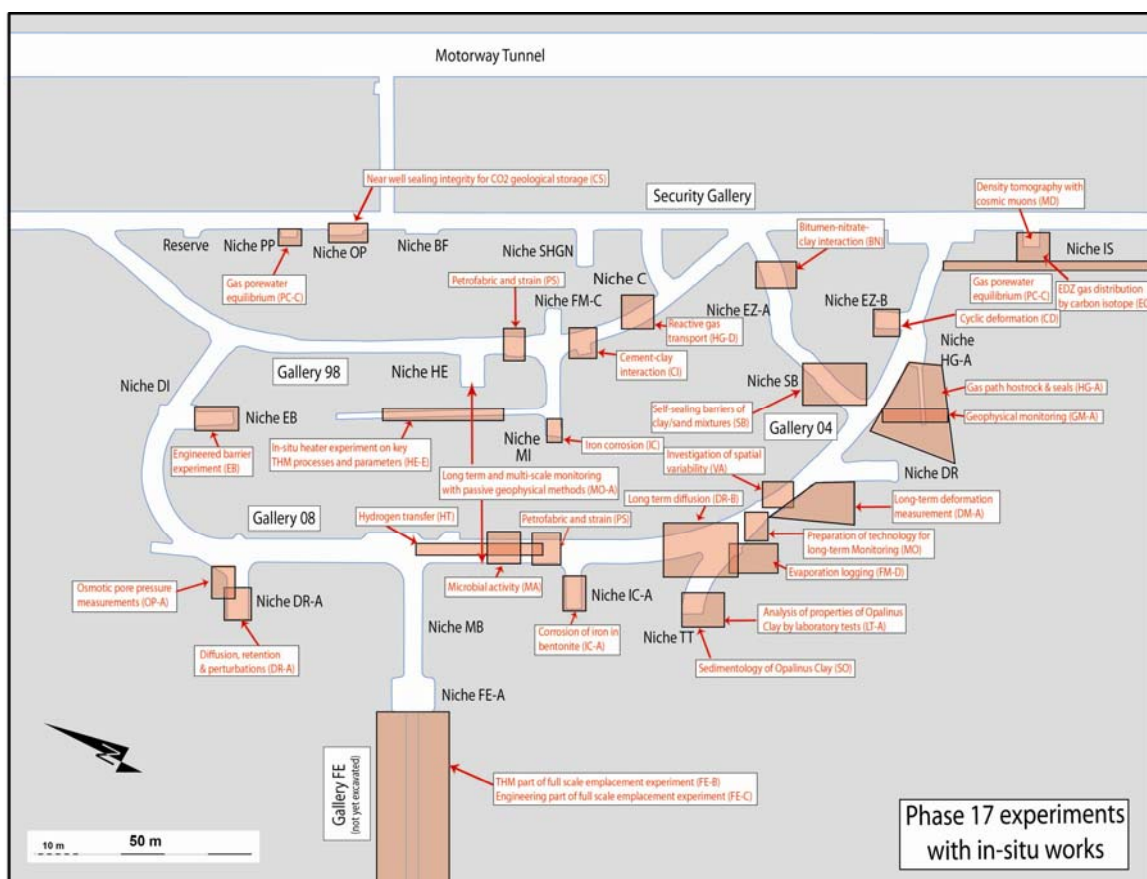




„4 Key-Results“

- High retention capacity
- Very low hydraulic conductivity
- Transport: Molecular diffusion
- Self-sealing

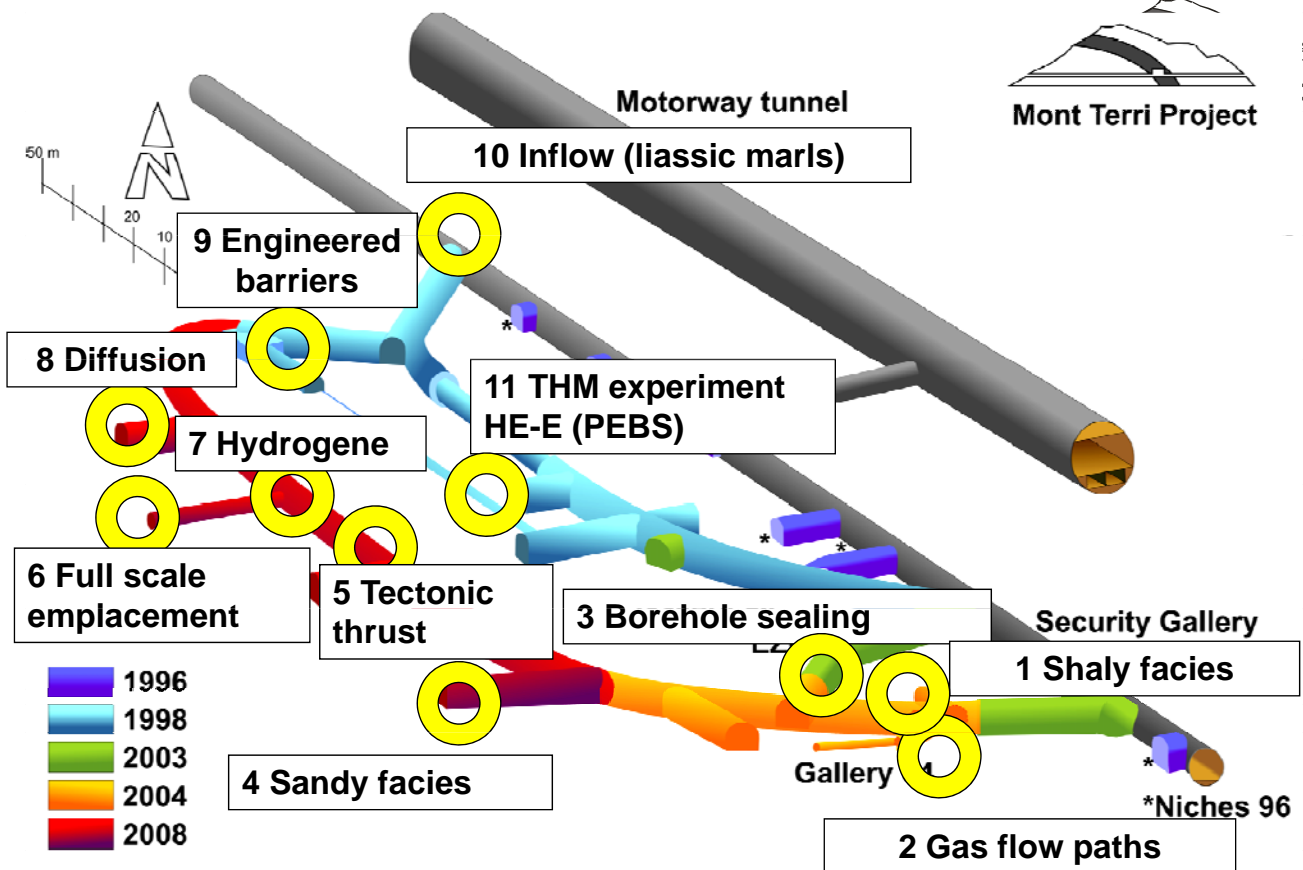
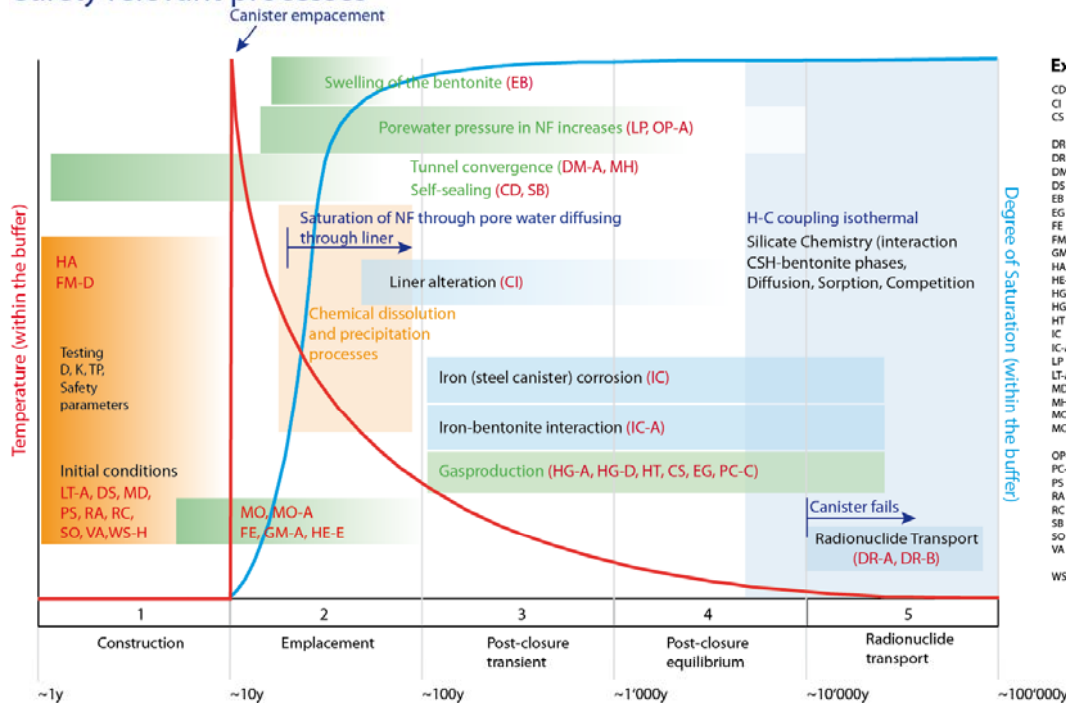
Ongoing experiments (1 of 2)





Repository evolution

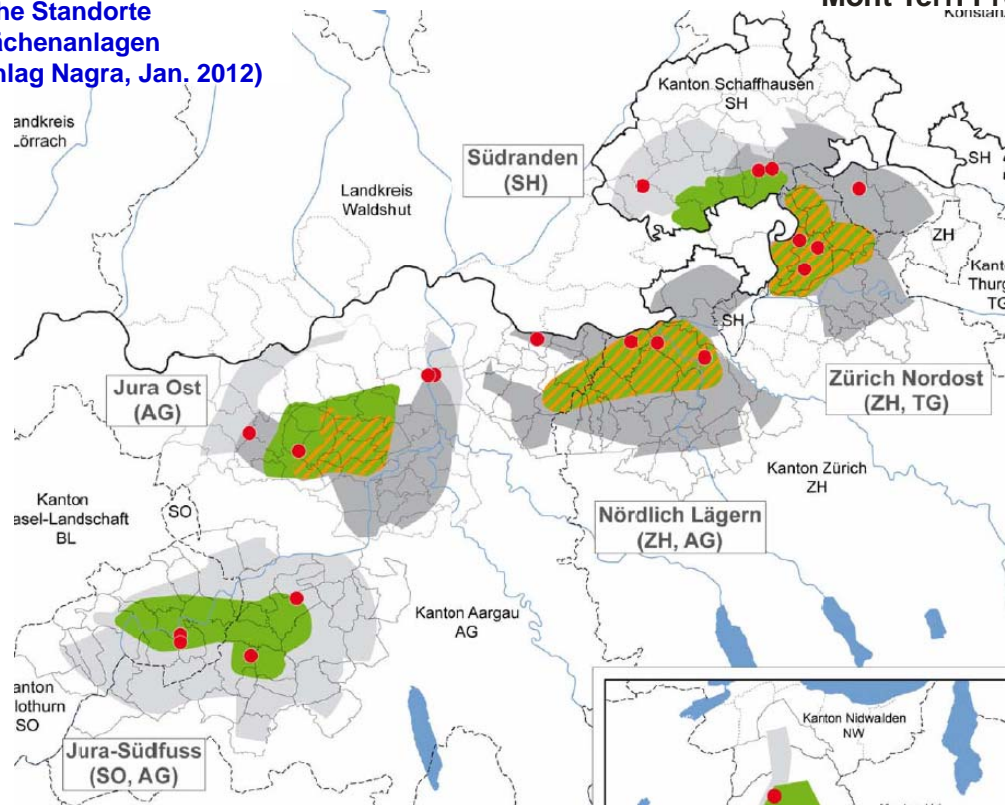
Safety relevant processes





Where? Sectorial plan

Mögliche Standorte
Oberflächenanlagen
(Vorschlag Nagra, Jan. 2012)



15

15



Conclusions

- The Mont Terri project is a scientific and technological platform for geological disposal in argillaceous formations
- 15 Partners from CH, EU, Japan, Canada and USA are participating: ANDRA, BGR, CHEVRON, CRIEPI, DOE, ENRESA, ENSI, GRS, IRSN, JAEA, NAGRA, NWMO, OBAYASHI, SCKCEN, SWISSTOPO. Sharing of knowledge and costs
- The Mont Terri rock laboratory contributes considerably to the safety and technical feasibility of a future Swiss repository for high-level waste in the Opalinus Clay.
- Where to store: a sectorial plan under the lead of the Federal Office of Energy is now running. 6 sites have been proposed by Nagra. Time schedule: authorisation not expected before 2025. Last word: Swiss population, national referendum.

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15



- Wear a helmet
- Transport with minibus
- Overpressure in rock laboratory (50 Pa)
- Security person: in case of emergency please follow her orders.



PEBS Workshop for Regulatory Authorities

St. Ursanne, April 25th and 26th, 2012

PEBS general overview, objectives, management

Michael Mente, BGR, Hannover Germany



Fig. 1

April 25th and 26th, 2012

Regulatory Authority Workshop



Presentation outline



Content

PEBS, the project objectives and the organisation

1. Short Presentation of the essential content of the Work Packages
 - scientific objectives
 - main challenges and milestones ahead
 - Composition of Consortium, Project organisation, Decision making
 - Website address of the project
2. Networking in the team and external integration
3. Financial and human resources involved
4. Expected impact on stakeholders
5. Society (nuclear regulatory requirements ?)

The Workshop, content and Objectives

6. Frame of Workshop

Fig. 2

April 25th and 26th, 2012

Regulatory Authority Workshop



1. Short Presentation of the essential content of the Work Packages

1. Work Package 1, SKB, Patrik Sellin
2. Work Package 2, ENRESA, Juan-Calos Mayor Zurdo
3. Work Package 3, GRS, Klaus Wieczorek
4. Work Package 4, NAGRA, Lawrence Johnson
5. Work Package B, BRIUG, Ju Wang, Liu Yuemiao
6. Work Package 5, BGR, Michael Mente
7. Work Package 6, BGR, Michael Mente

Fig. 3

April 25th and 26th, 2012

Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

Work Package 1, SKB, Patrik Sellin

Analysis of system evolution during early post closure period:
Impact on long-term safety functions

D1.1 and D1.2:

List of issues

List of scenarios and cases to be studied

Fig. 4

April 25th and 26th, 2012

Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

Work Package 2, ENRESA, Juan-Calos Mayor

Experimentation on key EBS processes and parameters

Task 2.1, Experimentation on key HM processes and parameters

Task 2.2, Experimentation on key THM processes and parameters

Task 2.3, Experimentation on key THM-C processes and parameters

Fig. 5

April 25th and 26th, 2012

Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

Work Package 3, GRS, Klaus Wiczorek

Modelling of short-term effects and extrapolation to long- term evolution

Task 3.1, HM modelling of the Mont Terri Engineered Barrier (EB) Experiment

Task 3.2, THM modelling for the planned heater test HE-E

Task 3.3, THM modelling of bentonite buffer

Task 3.4, Modelling of THM-C experiments on bentonite buffer

Task 3.5, Extrapolation to repository long term evolution

Fig. 6

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1. Short Presentation of the essential content of the Work Packages

Work Package 4, NAGRA, Lawrence Johnson

Analysis of impact on long-term safety and guidance for
repository design and construction

Fig. 7

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Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

Work Package B, BRIUG, Ju Wang, Yuemiao Liu

China mock-up test on compacted bentonite-buffer

Fig. 8

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Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

Work Package 5, BGR, Michael Mente

Dissemination

Fig. 9

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1. Short Presentation of the essential content of the Work Packages

Work Package 5: Dissemination I

Preparation and operation of a website

URL: <http://www.pebs-eu.de>

Preparation of a newsletter

Content:

- Proposed work, description of work of partner, objectives (1st Newsletter)
- Achieved results of partners or joint work (following newsletters)
- Events related to PEBS and related to other projects.....

Fig. 10

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Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

Work Package 5: Dissemination II

Workshops

- Open Bentonite workshop
- Bentonite training
- Two Special workshop for Regulatory Authorities
- Final workshop

Presentations at conferences

- Euradwaste....
- ANDRA conference Clays in natural & engineered barriers for radioactive confinement

Training and excursion

- Bentonite training
- Field trip to Bentonite producer

Fig. 11

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Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

Work Package 6, BGR, Michael Mente

Project Management

Fig. 12

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1. Short Presentation of the essential content of the Work Packages

Project organisation, decision making

1. Steering Committee: All WP Leader
2. Executive Committee (ExCom) All Partner (each partner with one vote)
3. High Level Expert Committee (HLEC), international external experts from different organisations with different roles

Fig. 13

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Regulatory Authority Workshop

1. Short Presentation of the essential content of the Work Packages

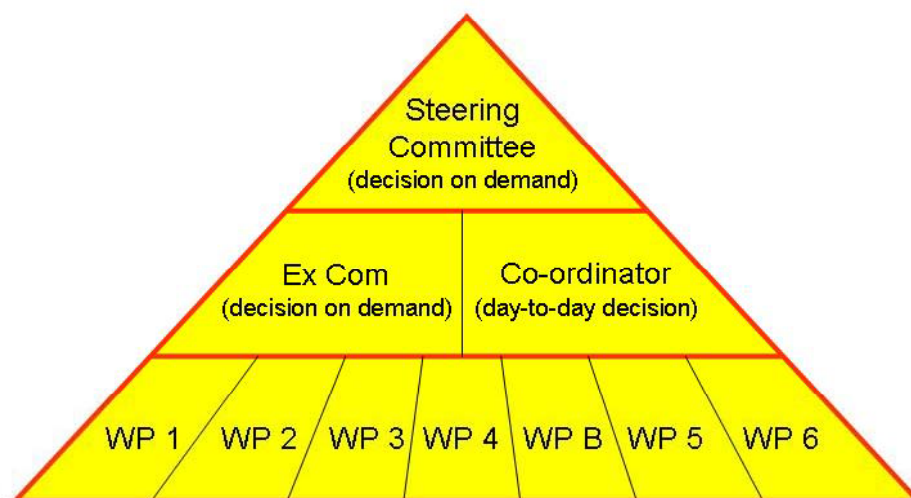


Fig. 14

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2. Networking in the team and external integration

Objective of an effective project team structure Individual skills and objectives

- Governmental own research **Increase independent knowledge**
- Industry **Products to meet customers demand**
- Consultant Companies **effective and flexible support to clients**
- Public Offices/Agencies **Follow the state of the art**
- Universities **Innovative ideas/prototypes but also training**
- Research Centres **Intensive lab works to qualify ideas**

Fig. 15

April 25th and 26th, 2012

Regulatory Authority Workshop

3. Financial and human resources involved

| Staff months: | Costs (in €): | Costs (only BRIUG in €): | Costs (only JAEA in €): |
|-------------------|-------------------|--------------------------|-------------------------|
| WP1: 5,75 | WP 1: 126.467,- | WP 1: | WP 1: |
| WP2: 210,32+4 | WP 2: 3.179.217,- | WP 2: 15.452,- | WP 2: |
| WP3: 83,11+4+8 | WP 3: 1.048.502,- | WP 3: 15.452,- | WP 3: 73.456,- |
| WP4: 11,75 | WP 4: 195.480,- | WP 4: | WP 4: |
| WPB: 180 | WP B: | WP B: 1.155.096,- | WP B: |
| WP5: 40+0,5 | WP 5: 474.260,- | WP 5: | WP 5: 3.028 |
| WP6: 18 | WP 6: 238.600,- | WP 6: | WP 6: |
| Total: 365,93 | Total: 5.262.525 | Total: 1.186.000,- | Total: 76.484,- |
| Incl. all: 562,43 | | | |

Red: BRIUG
Green: JAEA

Over all costs: 6.525.008,80 €
EC Contribution: 2.806.332,00 €

Fig. 16

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Regulatory Authority Workshop

Impact on

- Waste management organisations (implementers operators),
- Licensing
- Regulatory Authorities (state of the art)
- Mining industry and geology (information for planning, engineering, construction and implementation of final repositories seems to be quite fundamental)
- Science, research organisations
- Other stakeholders (Government, Policy, NGOs, public.....), independant knowledge, standards, rules,

Fig. 17

April 25th and 26th, 2012

Regulatory Authority Workshop

5. Society (nuclear regulatory requirements ?)

Impact on societal benefit areas:

- Safer facilities and increase expertise will **increase acceptance** for a repository (complete society will profit from the results)
- Appropriate dimension and construction of the repository (this will **reduce unnecessary costs**)
- Clear knowledge about the behavior of the repository allows exact monitoring (this will **increase confidence**)

Fig. 18

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Regulatory Authority Workshop

6. Frame of Workshop

This Workshop is proposed as a platform for the presentation of actual concepts, cutting edge methods and first results from running experiments

- Discussion and analysis of Identified important processes (FEPs) during the early evolution of the EBS
- Discussion of the results of the current treatment of the early evolution of the EBS in long-term safety assessments for spent nuclear fuel
- Discuss how the short-term transients will/may affect the long-term performance and the safety functions of the repository.
- Discussion of merits and shortcomings of the current treatment
- Discussion of future assessments related to events in the early evolution of the EBS.

Fig. 19

April 25th and 26th, 2012

Regulatory Authority Workshop

6. Frame of Workshop

In addition to the content of this workshop a second workshop is proposed for the end of the project what reflects both the final results of WP1 and WP 4 and includes:

1. Discussion the findings
 - of the WP2 and WP3 experiments and models,
 - of development of a more complete qualitative process-related description of the early evolution phase of the repository (the first several hundred years) and the residual uncertainties in the evolution,
 - of possible different behaviours of the system that may be implied by the uncertainties or disagreement between models and experiments

Fig. 20

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Regulatory Authority Workshop

6. Frame of Workshop

2. Presentation and discussion of the results of experiments and models and their significance in relation to long-term safety functions of the buffer, canister and host rock (clay and crystalline) in a quantitative fashion, including the importance of residual uncertainties
 - importance of the transient period with regard to the long-term characteristics particularly relevant to system performance and long-term safety;
 - of uncertainties arising from disagreement between models and experiments and their implications for extrapolation of results, with particular emphasis on possible impacts on safety functions.
3. Presentation of an improved and more complete approach to integrating the thermal and resaturation phase of the repository with the long-term steady state phase of repository evolution.

Fig. 21

April 25th and 26th, 2012

Regulatory Authority Workshop

The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 249681”

Fig. 22

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Regulatory Authority Workshop

Thank you for your attention!



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PEBS website: <http://www.pebs-eu.de>

EU Euratom website: http://ec.europa.eu/energy/nuclear/euratom/euratom_en.htm

BGR website: <http://www.bgr.bund.de>

Fig. 23

April 25th and 26th, 2012

Regulatory Authority Workshop

Overview and current results of:
Work package 1 (Analysis of system evolution during early post-closure
period, Impact on long-term safety functions)
Work package 4 (Analysis of impact on long term safety)

Patrik Sellin SKB

Lawrence Johnson, Nagra



Participants

- BGR
- NAGRA
- SKB
- ENRESA
- ANDRA
- GRS (WP4)

Outline

- WP1 Objectives
- WP1 Report
- WP4 Objectives
- WP4 Cases

WP1 - Objectives

- Identify important processes during the early evolution of the EBS
- Describe the current treatment of the early evolution of the EBS in long-term safety assessments for spent nuclear fuel/HLW
- Discuss how the short-term transients will/may affect the long-term performance and the safety functions of the repository.
- Identify the merits and shortcomings of the current treatment
- Discuss the needs for additional studies of these issues and how they can support future assessments – give directions to other WPs
- Define “scenarios” related to events in the early evolution of the EBS

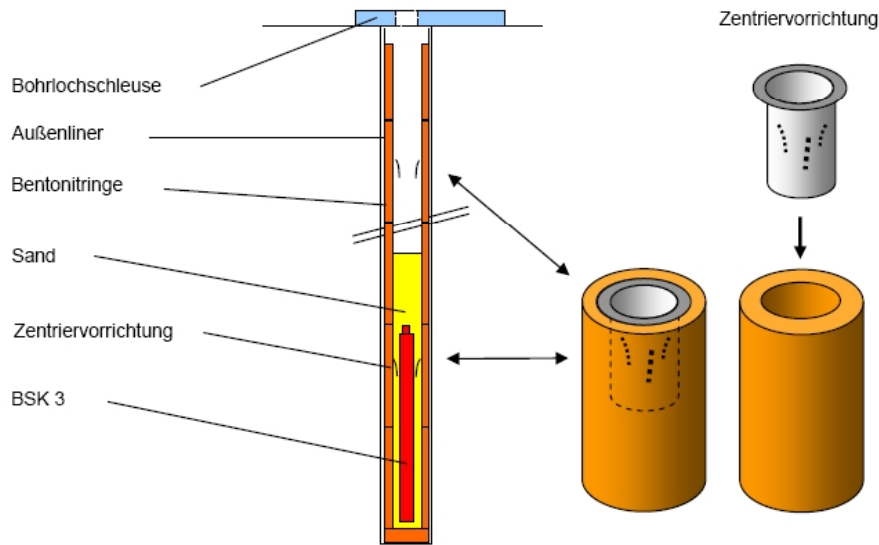
WP1 Report

- The PEBS project
- Analysis of system evolution during early post closure period: Impact on long-term safety functions
- The current treatment of the early evolution of the EBS in long-term safety assessments for spent nuclear fuel/HLW in 5 national programmes
 - Repository concept
 - Safety assessment methodology
 - Safety functions
 - Early evolution of the EBS
 - Identified uncertainties ([Deliverable D1](#))
- Definition of cases/scenarios to be studied ([Deliverable D2](#))
 - Water uptake in clay components of the EBS
 - Mechanical evolution
 - Alteration of the hydro-mechanical properties
- Cases to be studied in PEBS
- Preliminary version of the report available on the website
 - >90 pages

WP1 Report

- Repository concept
- Safety assessment methodology
- Safety functions
- Early evolution of the EBS
- Identified uncertainties

Repository concept

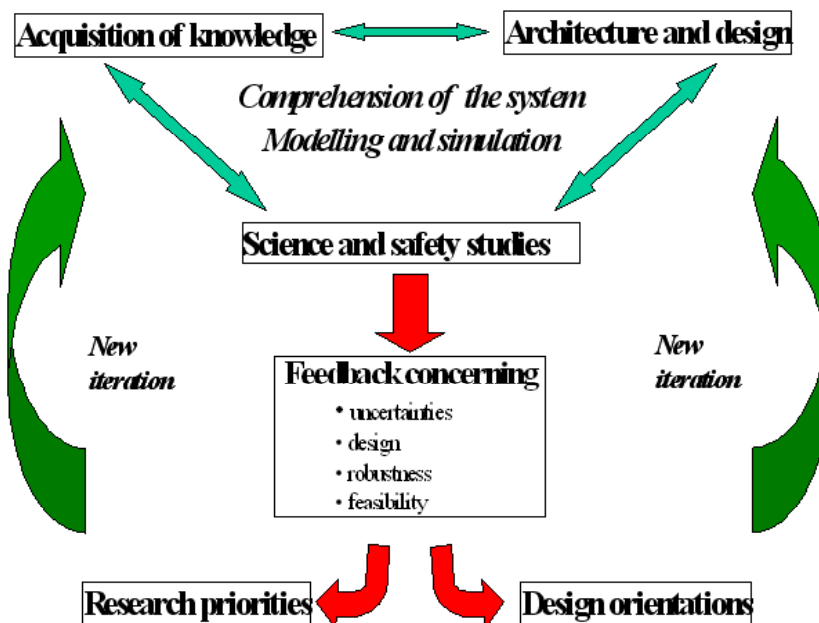


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Safety assessment methodology



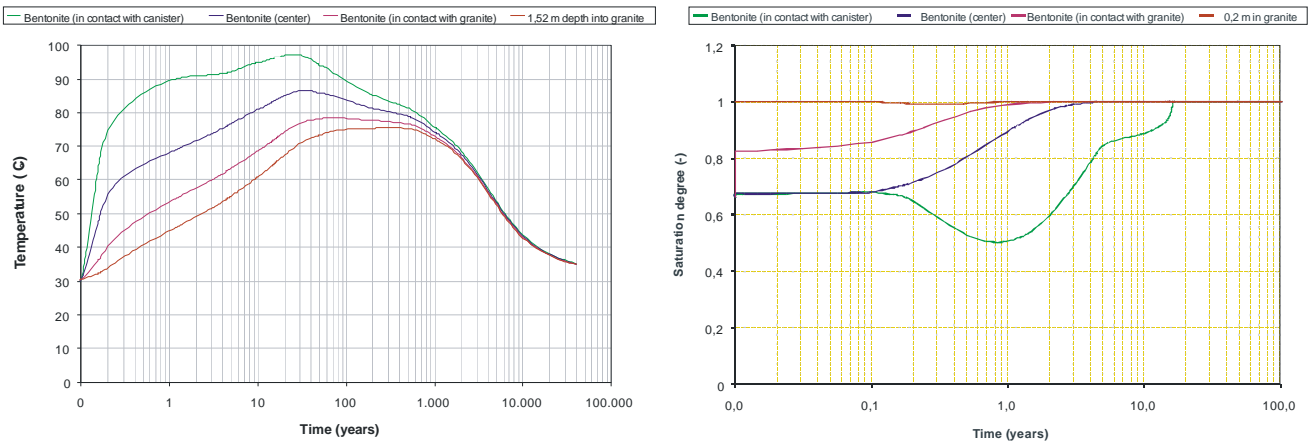
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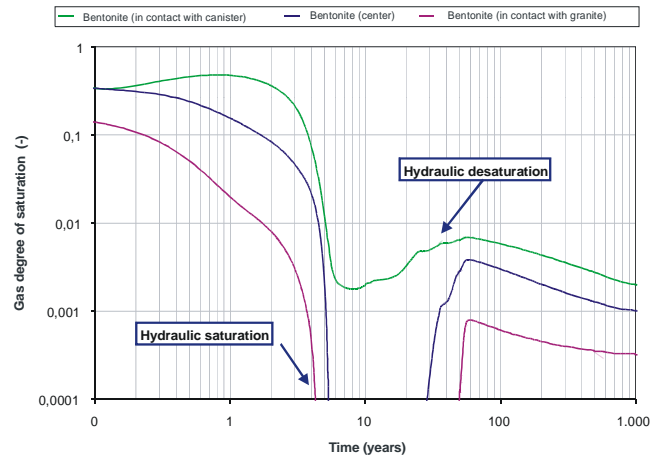
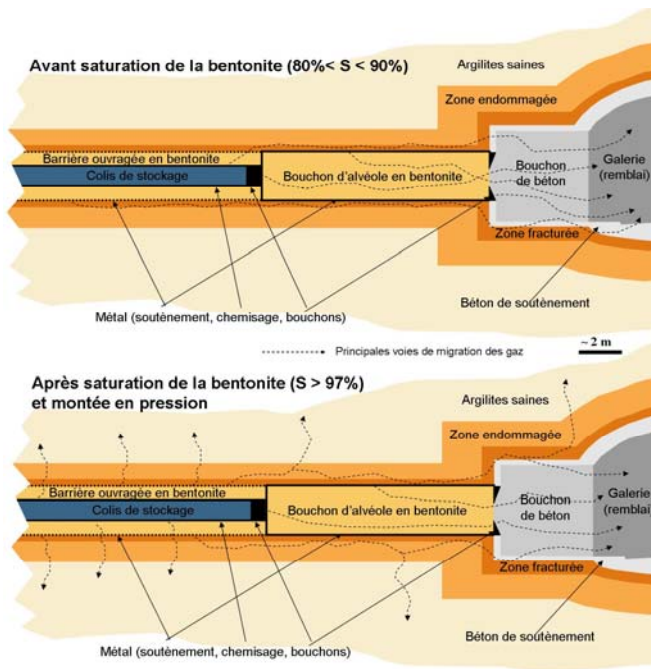
| Safety-relevant attributes | Favours/contributes to ... | Performance indicator |
|--------------------------------------|--|--|
| Low hydraulic conductivity | Attenuation safety function of buffer, by ensuring diffusive transport | $K < 10^{-12} \text{ m s}^{-1}$ for hydraulic seal $K < 10^{-11} \text{ m s}^{-1}$ for buffer around canister |
| Chemical retention of radionuclides | Attenuation safety function of buffer, by retarding transport from the buffer | No quantitative criterion, strong sorption is favored |
| Sufficient density | Attenuation safety function of buffer, by preventing colloid transport | $\rho_s > 1650 \text{ Mg m}^{-3}$ |
| Sufficient swelling pressure | Attenuation safety function of rock, by providing mechanical stabilization of rooms, and hence avoiding significant extension of EDZ | $0.6 \text{ MPa} < P_s < \text{minimum principal stress}$ $\rho_s > 1750 \text{ Mg m}^{-3}$ |
| | Containment safety function of canister, by ensuring it is surrounded by a protective layer of buffer (stress buffering) | $0.2 \text{ MPa} < P_s < \text{minimum principal stress of rock}$ - canister has to be designed to be robust enough to take up the deformation - buffer must be sufficiently viscous to avoid canister sinking |
| Sufficient gas transport capacity | Attenuation safety function of buffer, by ensuring gas can migrate without compromising hydraulic barrier | No quantitative criterion (less than the minimum principal stress) |
| Minimize microbial corrosion | Containment safety function of canister, by ensuring conditions favorable to slow corrosion | No quantitative criterion (density should be high) |
| Resistance to mineral transformation | Ensuring the required long-term stability, by providing longevity of safety-relevant attributes of buffer | No quantitative criterion |
| | Containment safety function of canister, by providing stress buffering | No quantitative criterion |
| Suitable heat conduction | Containment safety function of canister, by ensuring favorable maximum temperature conditions | $0.4 < T_c < 2 \text{ W m}^{-1} \text{ K}^{-1}$ (for a specific thermal heat load of 1500 W) |
| | Safety functions of buffer and rock, by ensuring favorable maximum temperature conditions | $0.4 < T_c < 2 \text{ W m}^{-1} \text{ K}^{-1}$ (for a specific thermal heat load of 1500 W) |

Early evolution of the EBS



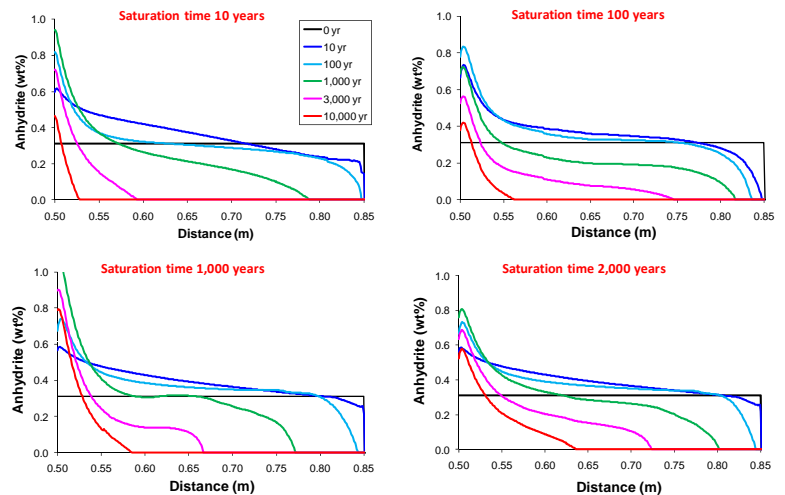
THM-Evolution

Early evolution of the EBS

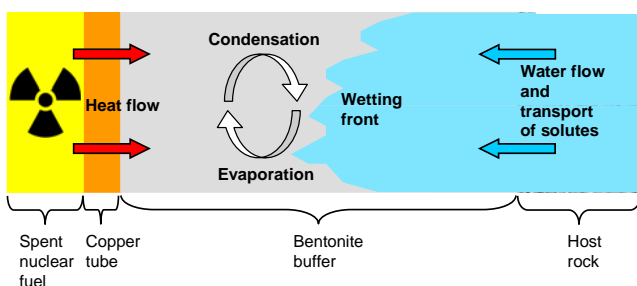


Gas evolution

Early evolution of the EBS



Chemical evolution



Identified uncertainties

- Mass loss due to piping and erosion in the very early evolution
- Swelling and homogenisation of components with different density and sealing after losses of mass
- The importance of friction within the bentonite and between bentonite and other materials – also in the unsaturated state
- Effects of temperature on the mechanical properties
- Hydraulic processes
- Mechanical behavior in contact with the metal elements
- Mechanical effect of gases inside Argillites and swelling clay
- Thermo-mechanical effects
- Technologies implemented in the repository: swelling clay seals and engineered barriers
- The effect of temperatures exceeding 100°C on the hydraulic properties of the buffer
- The evolution of swelling pressure with time and the interaction with the convergence of the host rock
- Chemical Interaction between bentonite and Fe and the low pH liner
- Discrepancy in the water saturation process of the buffer between predicted hydration rates and experimental values

Definition of cases/scenarios to be studied

- Water uptake in clay components of the EBS
- Mechanical evolution
- Alteration of the hydro-mechanical properties

Cases to be studied in PEBS

- Will be based on *cases/scenarios*
- Needs to be of general interest
- Needs to relate to studies performed within the project
 - Use of data and observations from the project
- Possible to evaluate within the project

WP4 - Objectives

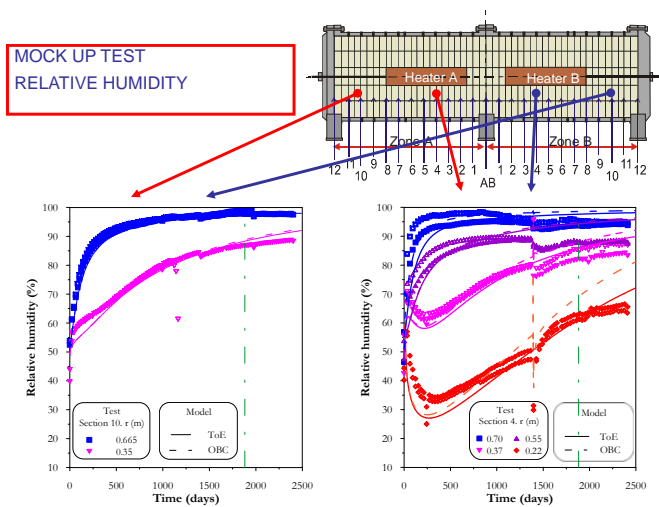
- Obtain an overview of the findings of PEBS and relate the results and uncertainties to the long-term safety functions of the repository components
- Provide a more complete description of the THMC evolution of the near field
- Give some guidance regarding repository design, by clarifying the link between long-term safety criteria and design criteria of the EBS

Cases for the purpose of WP4

- Case 1. Uncertainty in water uptake in buffer ($T < 100^\circ\text{C}$)
 - Origin – standard THM model vs. FEBEX observations
 - PEBS: new modelling and FEBEX mock-up data etc.
- Case 2. Uncertainty in T evolution in buffer ($T > 100^\circ\text{C}$)
 - Origin – lack of validation of TH model for high T and low saturation rate
 - PEBS: HE-E experiment modelling and exp. results
- Case 3. Uncertainty in HM evolution of buffer
 - Origin – lack of large-scale experiments
 - PEBS: EB experiment results
- Case 4. Uncertainties in chemical evolution
 - Origin – experiments vs. models of corrosion product/bent and cement/bentonite interactions
 - PEBS – GAME experiments and modelling

Case 1. Uncertainty in water uptake in buffer ($T < 100^\circ\text{C}$)

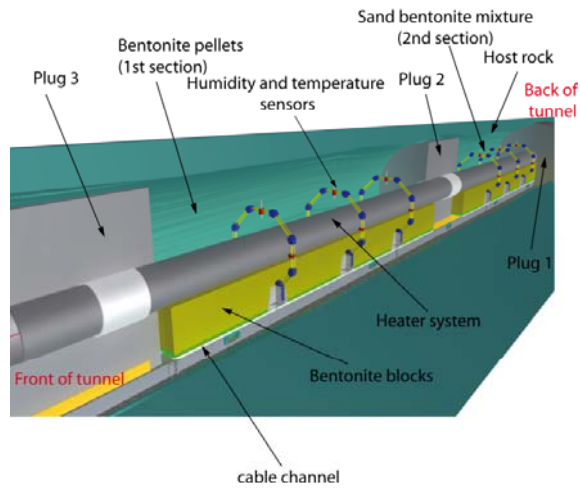
- Activities within PEBS:
 - Uncertainty assessment (Modelling)
 - FEBEX mock-up data and modelling
 - THM Column Tests at Ciemat
 - EB experiment
 - FEBEX in situ test and modelling
- Variant cases:
 - Isothermal saturation (extrapolation to seal performance)
 - Long term FEBEX in situ with constant T of 100°C
 - Long term extrapolation using realistic thermal source term



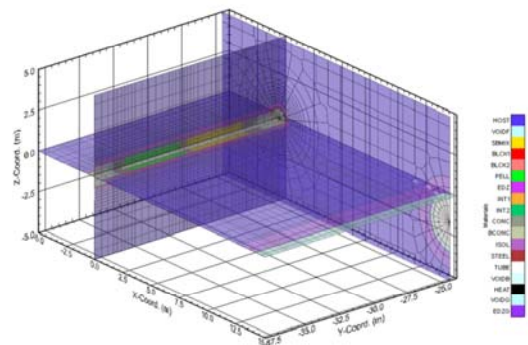
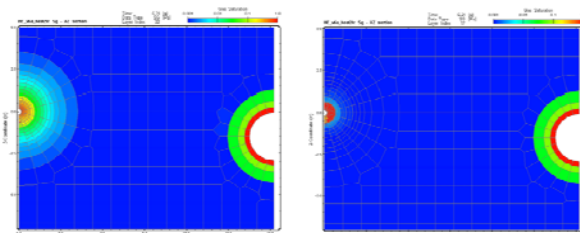
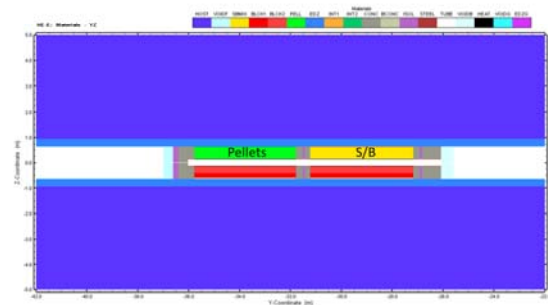
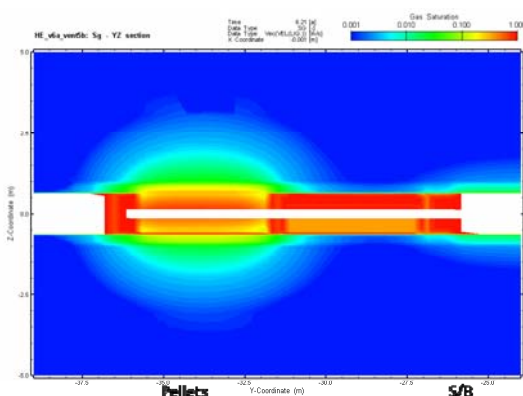
Measured and calculated relative humidity in the FEBEX mock-up taking into account thermo-osmosis

Case 2. Uncertainty in T evolution in buffer (T >100°C)

- Activities within PEBS:
 - HE-E experiment and modelling
- Variant cases:
 - Long term extrapolation using real thermal source term

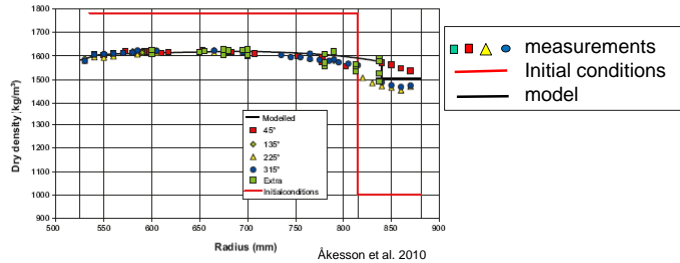


TOUGH (TH): first predictive calculations – as-built data



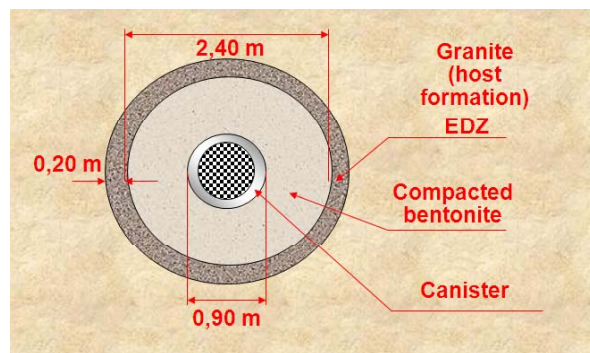
Case 3. Uncertainty in HM evolution of buffer

- Activities within PEBS:
 - EB experiment and modelling
 - HE-E experiment and modelling
 - Febex mock-up and in situ
 - Stress-strain behaviour studies
- Variant cases:
 - Uncertainty in HM evolution of buffer (pellets)
 - Impact of heat on the HM properties
 - Hydromechanical impact from corrosion processes (feedback from case 4)

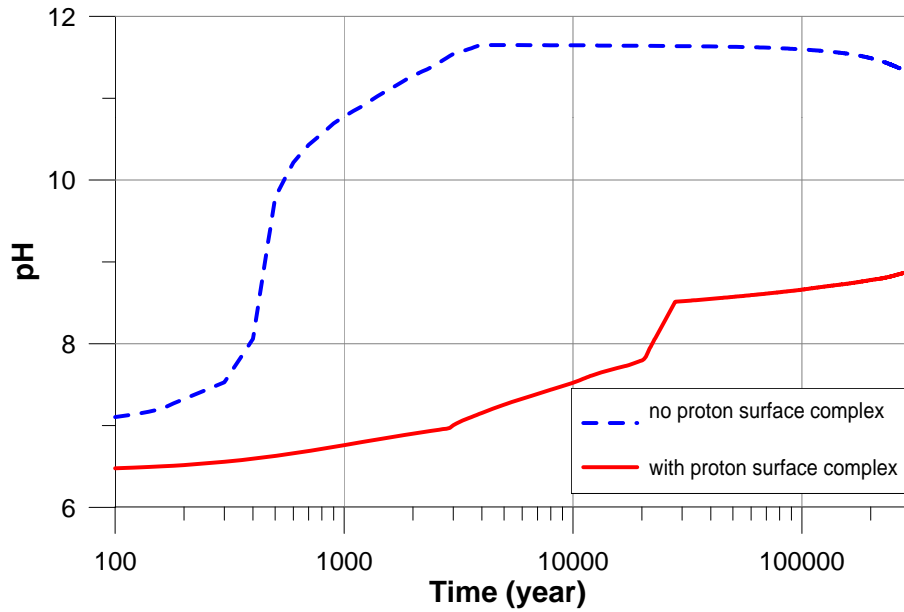


Case 4. Uncertainties in chemical evolution

- Activities within PEBS:
 - GAME experiments and modelling
 - Interface studies
 - Modelling
- Variant cases:
 - Study of the canister/bentonite interfaces
 - Study on the concrete/bentonite interfaces
 - Long term evolution in the granite



pH in bentonite: sensitivity to surface complexation



“The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 249681”

Patrik Sellin

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Overview of Work Package 2 “Experimentation on key EBS processes and parameters”

Juan Carlos Mayor, Enresa



26 April 2012

PEBS Workshop

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Outline

- Participants
- Objectives
- Methodological approach
- Organization in tasks
- Activities per task
- Summary

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WP2 Participants

BGR, G

GRS, G

ENRESA, E

AITEMIN, E

CIEMAT, E

GOLDER, E

UAM, E

NAGRA, CH

Solexperts, CH

Clay Technology, S

SKB, S

ANDRA, F

BRIUG, China

WP2 - Objectives

- Evaluation of the key Thermal, Hydraulic, Mechanical and Chemical processes and parameters during the early evolution of the EBS system, as identified in WP1
- Provide with a reliable good quality experimental data base, including different time and spatial scales, as input to:
 - The modelling and extrapolation work (WP3)
 - The analysis of the impact of uncertainties on long-term safety (WP4)

WP 2: Methodological Approach

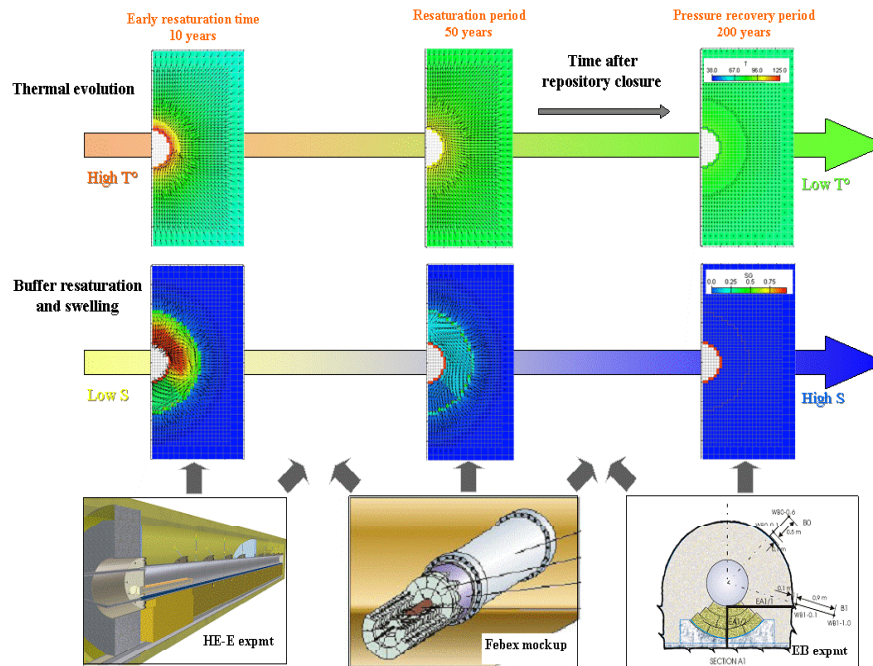
- Performing experiments, including different time and spatial scales, according to the needs for additional modeling studies on key processes during the early EBS evolution which still exhibit some remaining uncertainties
- Making use to the extent possible of on going experiments being conducted by the PEBS team (in the laboratory and in situ)

Identified uncertainties (WP1)

addressed in WP2 work

- Mass loss due to piping and erosion in the very early evolution
- Swelling and homogenisation of components with different density and sealing after losses of mass
- The importance of friction within the bentonite and between bentonite and other materials – also in the unsaturated state
- Effects of temperature on the mechanical properties
- Hydraulic processes
- Mechanical behavior in contact with the metal elements
- Mechanical effect of gases inside Argillites and swelling clay
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- Technologies implemented in the repository: swelling clay seals and engineered barriers
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- The evolution of swelling pressure with time and the interaction with the convergence of the host rock
- Chemical Interaction between bentonite and Fe and the high pH liner
- Discrepancy in the water saturation process of the buffer between predicted hydration rates and experimental values

Concept of the validation experiments in the project PEBS



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WP 2: Organization in tasks

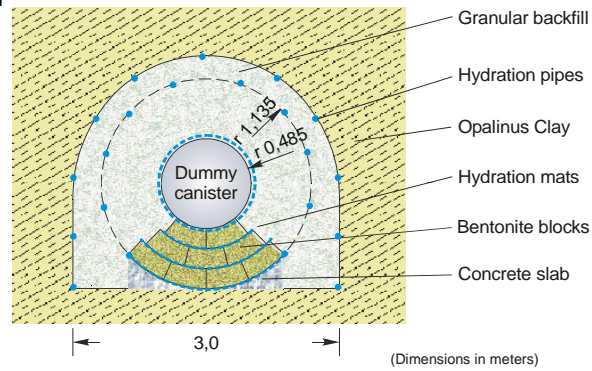
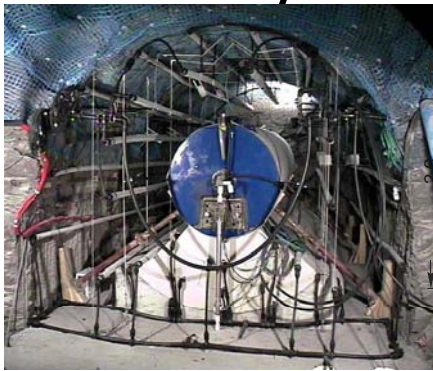
1. **Task 2.1. Experimentation on key HM processes**
 1. Laboratory infiltration tests
 2. EB *in-situ* experiment
2. **Task 2.2. Experimentation on key THM processes**
 1. Subtask 2.2.1 Laboratory experimentation on key THM processes
 1. The FEBEX mock-up
 2. Long-term tests in cells simulating particular disposal concepts
 3. Studies on stress-strain behavior
 2. Subtask 2.2.2 *In-situ* experimentation on key THM processes
3. **Task 2.3. Experimentation on key THM-C processes**
 1. Subtask 2.3.1 THM-C mock-ups (GAME)
 2. Subtask 2.3.2 THM & THM-C tests on key processes at the interfaces
 1. Study of the corrosion processes at the canister/bentonite interface
 2. Study of the processes at the concrete/compacted bentonite interface

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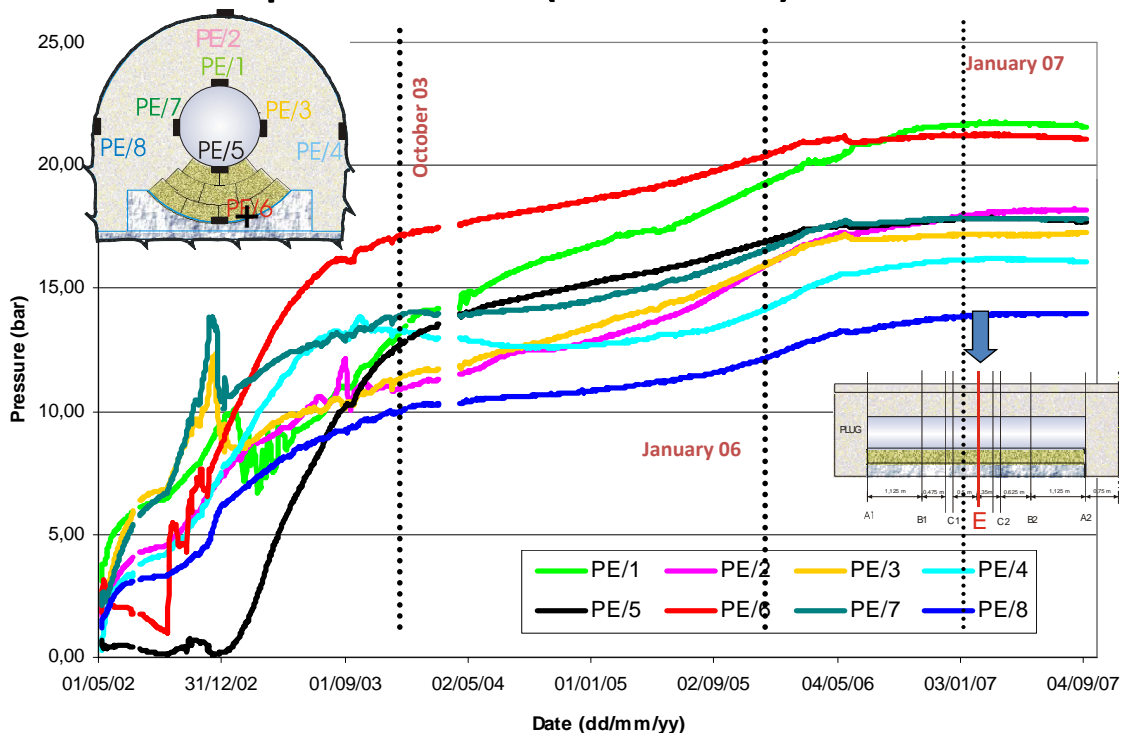
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Task 2.1 Experimentation on key HM processes



- Laboratory infiltration tests:** isothermal saturation of mixtures of bentonite pellets with water injected at low pressure (The water intake and the swelling pressure are measured precisely) to complete knowledge on the hydration and swelling process.
- EB in-situ experiment :** Controlled dismantling to complete knowledge on the resaturation and swelling processes of the of the EB bentonite buffer, which artificial hydration process started back in May 2002. Determine the hydraulic conductivity of the emplaced buffer (after its saturation in-situ) and its achieved degree of homogeneity, in order to demonstrate that the hydraulic conductivity is low enough and not too heterogeneous.

EB experiment: total pressure (Buffer)



Task 2.1 Experimentation on key HM processes

Main tasks of the EB in-situ experiment

1. Perform an extensive “in situ” sampling and analysis of the actual state of the clay barrier (Autmun 2012)
2. Very big bentonite samples in order to determine their hydraulic conductivity, porosimetry, relevant mechanical properties and suction values.
3. Improve the analysis of the water balance of the experiment.
4. Investigation of the nature and evolution of EDZ in Opalinus Clay (seismic survey)
5. Recovery of some of the monitoring sensors, in order to analyze their performance.

Task 2.2 Experimentation on key THM processes

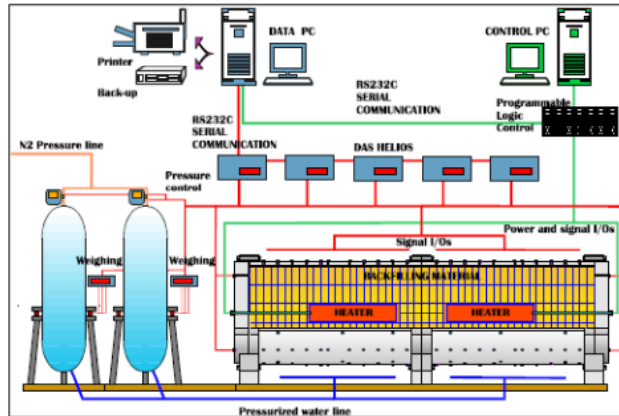
Subtask 2.2.1 Laboratory experimentation on key THM processes (I)

The FEBEX mock-up: some background

- Running since February 1997 as a fundamental component of the FEBEX experiment
- 2 heaters operating at constant power supply (700 W/heater), with T on the heaters surface close to 100 °C
- Overall degree of saturation is very high, about 97 %, but increasing very slowly
- More than 89 % of the total number of sensors remains operative, but this percentage is 93% for temperature, 75% for relative humidity (RH), 65% for fluid pressure, 71% for tangential pressure (PT), 71% for radial pressure (PR) and 82% for axial pressure (PZ).

Task 2.2 Experimentation on key THM processes

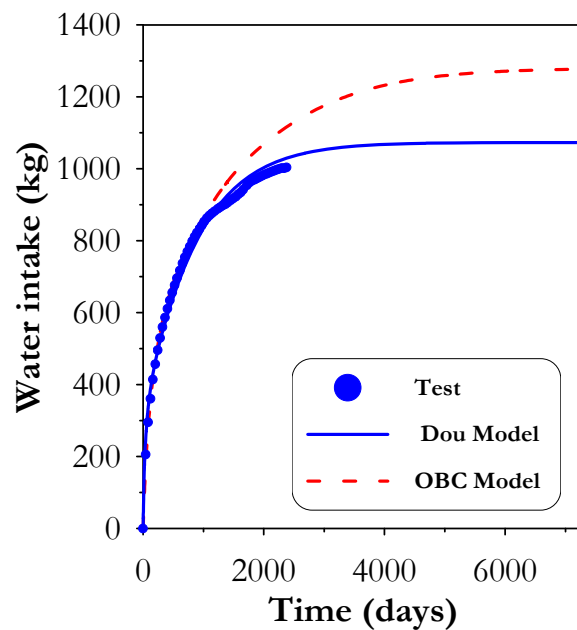
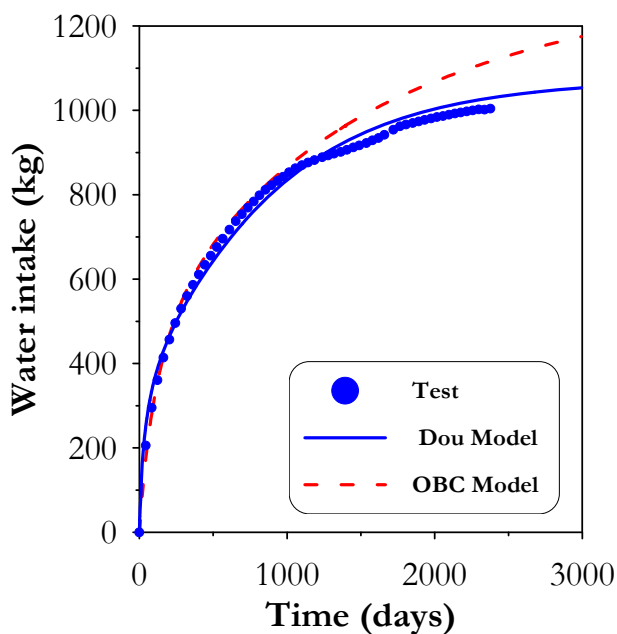
Subtask 2.2.1 Laboratory experimentation on key THM processes (II)



The FEBEX mock-up

- 1. Operation:** Continuation of the FEBEX “mock-up” operational phase in its present state.
- 2. Preparation of Sampling Book:** Specify the samples (location, type and number) to be taken in case of failure of the experiment to prevent losing THM information, as well as the tests to be performed.
- 3. Preparation of Database:** Compile and analyze existing information on backfill materials and in the evolution of the clay barrier subjected to thermal and hydraulic flows.

FEBEX mock-up: water inflow

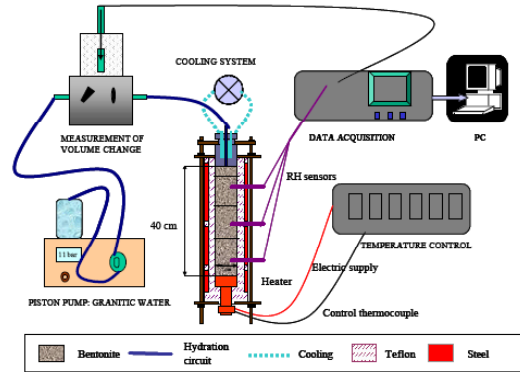


Task 2.2 Experimentation on key THM processes

Subtask 2.2.1 Laboratory experimentation on key THM processes (III)



Infiltration cells in operation: isothermal (left) and with thermal gradient (right)



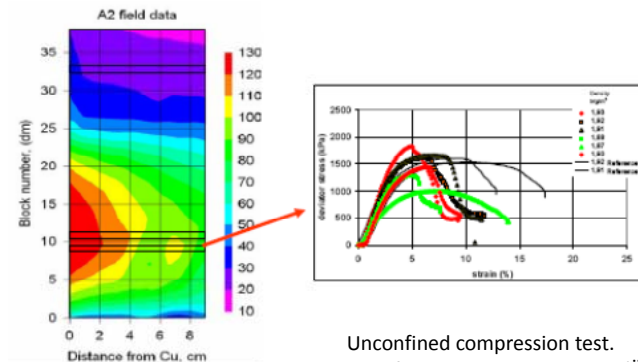
Experimental setup for the infiltration tests

Long-term tests in medium size cells

- 1. Tests already running:** Two infiltration tests being carried out since 2002 by CIEMAT, one of them is heated at the bottom at 100 °C and the other one performed at isothermal conditions
- 2. New tests:** with other materials (bentonite / sand mixtures) and using realistic repository-like heating rates, in support of HE-E

Task 2.2 Experimentation on key THM processes

Subtask 2.2.1 Laboratory experimentation on key THM processes (IV)



Unconfined compression test. Data from the LOT experiment (Äspö)

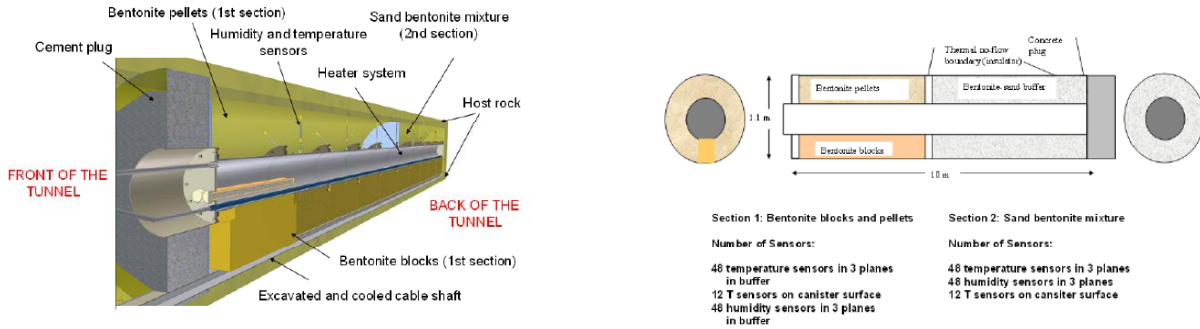
Studies on stress-strain behavior

Motivation: Significant lower strain at failure was measured in material exposed to high T (LOT exp.)

- 1. Unconfined compression tests:** to study the mechanical properties more in detail as a function of increased T, T gradient or other factors coupled to the exposure of increased temperature
- 2. Triaxial tests:** to determine on samples exposed to increased T: swelling pressure; water retention; and shear strength

Task 2.2 Experimentation on key THM processes

Subtask 2.2.2 In situ experimentation on key THM processes



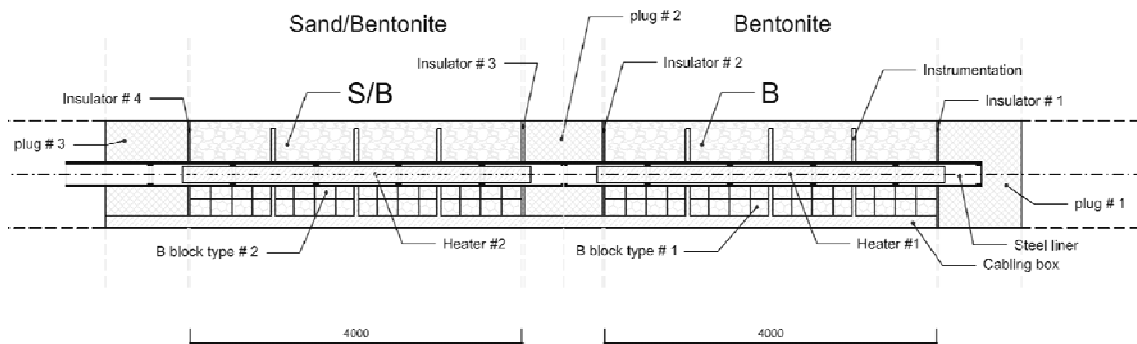
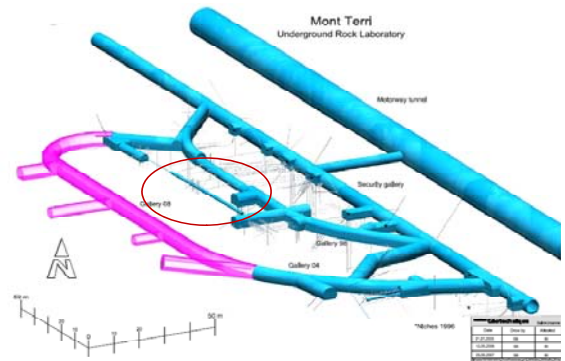
The new heater HE-E test is aimed at studying the thermal evolution of the near field around the canister during the very early phase after emplacement (the early non-isothermal resaturation period). A heater system, capable of representing the temperature curve of the anticipated heat production in the canisters (140°Cmax), is gradually leading to and increase in temperature in the EBS and the surrounding host rock while natural saturation is ongoing.

Specific objectives are:

- to provide the experimental data base required for the validation of existing thermo-hydraulic models of the early resaturation phase
- to upscale thermal conductivity of the partially saturated buffer from laboratory to field scale (pure bentonite and bentonite-sand mixtures)

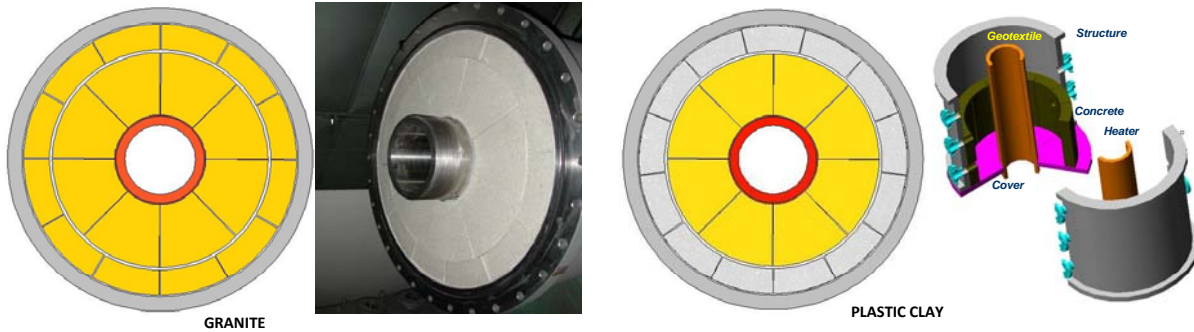
HE-E heater experiment

- 1:2 scale (microtunnel 1.3 m)
- Natural resaturation from clay hostrock
- Heater surface temperature: 140°C
- Duration: June 2011 - >2014
- Two symmetrical sections - different granular materials



Task 2.3 Experimentation on key THM-C processes

Subtask 2.3.1 THM-C mock-ups



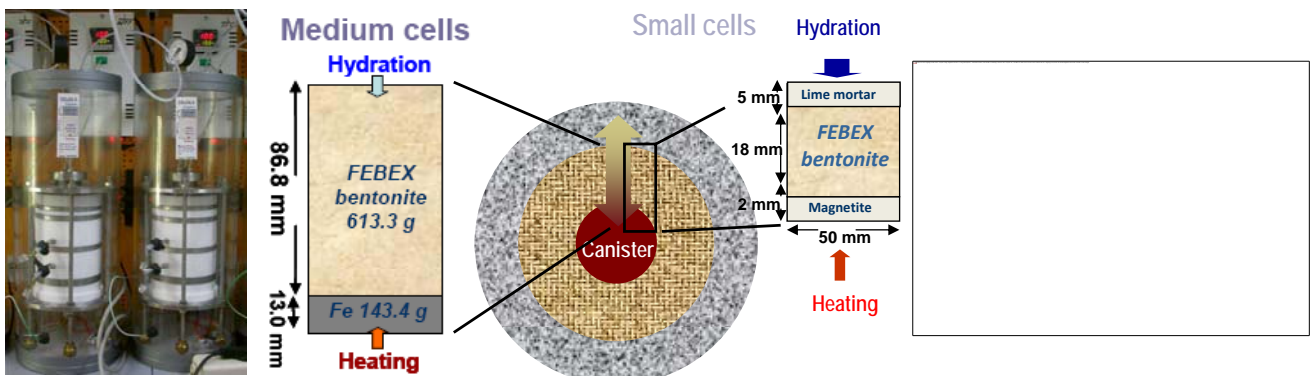
The THM-C mock-ups (GAME tests) simulate the components of the EBS in accordance with ENRESA's reference concepts to reproduce the expected conditions in the granitic and argillaceous geological repositories after their closure. Both mock-ups contain metal specimens and only one concrete blocks

The objectives are:

1. Research on the potential changes that may occur in the key parameters of the buffer material as a result of THM and THC processes.
2. Monitoring geochemical changes by sampling of pore water with the minimum possible interference with the system.

Task 2.3 Experimentation on key THM-C processes

Subtask 2.3.2 THM-C tests on key processes at the interfaces (I)



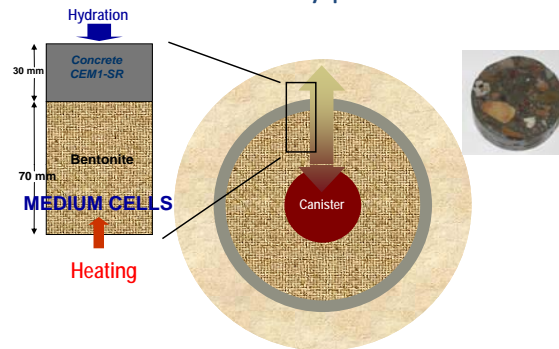
Study of the corrosion processes at the canister/bentonite interface:

Continuation of NF-PRO Project: Experiments at two scales (columns of 10 and 2.5 cm height) were performed, with duration from 3 weeks to 1.5 years, using either corrosion products or steel, with the aim of both study the corrosion products generated and their impact on bentonite properties (mineralogy, geochemistry, porosity, etc.)

PEBS Project:

- Four experiments in medium cells are still running; One was dismantled after 4 yrs and 5 months of operation and another one will be dismantled after 6 yrs and 8 months of operation. The other two will be left running until end of the project. The objective of the sequential dismantling is getting information on the geochemical evolution of the interface.
- New tests in small cells were set at the beginning of the project to study the combined interaction concrete/bentonite /steel by simulating the conditions expected after 1000-3000 years of repository operation.

Subtask 2.3.2 THM-C tests on key processes at the interfaces (II)



Study of the processes at the concrete/compacted bentonite interface:

Continuation of NF-PRO: short and medium-term (0.5 to 1.5 years) experiments at medium scale (10 cm) were run, dismantled and analyzed to provide experimental evidences on the physical, chemical and mineralogical changes due to the concrete-bentonite interaction.

PEBS Project:

Four experiments in medium cells (set during NF-PRO) are still in course. One of them was dismantled after 4 yrs and 7 months of operation and another one will be dismantled after 6 yrs and 10 months of operation. The third one will be left running during the whole duration of the project.

Expected outcome is:

- 1.The confirmation of the low impact of the alkaline plume in terms of the mineralogical alteration thickness
- 2.The precise establishment and evolution over time of the new formed by-products and how they produce a porosity reduction process affecting diffusive transport.

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Summary

- WP2 is a central part of the PEBS project from a technical and scientific point of view. It also consumes most of the human and economical resources of the project
- Experiments are running according to expectations. Explicit mention is made to the challenge of the HE-E new heater experiment
- WP2 is already providing with a reliable good quality experimental data base to the modeling activities in WP3
- Very good and close cooperation among “experimentalists” of WP2 and “modellers” of WP3

“The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 249681”

Juan Carlos Mayor

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ENRESA (Madrid, SPAIN)



PEBS Workshop for Regulatory Authorities

THM and THM-C laboratory experiments



St. Ursanne, April 25th and 26th, 2012



April, 25th and 26th 2012

Regulatory Authority Workshop



Tasks



- **T21. EXPERIMENTATION ON KEY HM PROCESSES AND PARAMETERS (in situ and laboratory)**
- **T221. LABORATORY EXPERIMENTATION ON KEY THM PROCESSES AND PARAMETERS (mock-up and laboratory)**
- **T231. THM-C MOCK-UPS (GAME TESTS)**
- **T232. THM AND THMC TESTS AIMED AT THE UNDERSTANDING OF KEY PROCESSES TAKING PLACE AT THE INTERFACES (laboratory)**

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| | FEBEX (granulated) | MX-80 (powder) |
|--|---|---|
| Mineralogy (%) | Montmorillonite (92±3), quartz, plagioclase, cristobalite | Montmorillonite (65-82), quartz, calcite, feldspars, pyrite |
| CEC (meq/100g) | 102±4 | 75-82 |
| Exchangeable cations (meq/100g) | Ca (35), Mg (31), Na (27), K (2.6) | Na (61), Ca (10), Mg (3) |
| Hygroscopic water content (%) | 13.7±1.3 | 8-11 |
| Liquid limit (%) | 102±4 | 350-570 |
| P_s for ρ_d 1.6 g/cm ³ (MPa) | 6 | 7 |
| Total specific surface (m ² /g) | 725±47 | 512 |

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T21. EXPERIMENTATION ON KEY HM PROCESSES AND PARAMETERS

AIMS

- Evaluate the key HM processes and parameters taking place during the early evolution of the EBS
- Provide a reliable good quality experimental HM data base, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3

ACTIVITIES (all of them at lab T)

- Infiltration test with EB FEBEX pellets
- Infiltration tests with HE-E materials
- Long-term infiltration tests with measurement of permeability at low hydraulic gradients (FEBEX and MX-80)



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Infiltration tests with FEBEX pellets

AIMS

- Provide support for the modelling of the **EB in situ test**
- Check the long-term hydro-mechanical behaviour of a pellets barrier
- Compare the HM behaviour of pellets and compacted bentonite

TESTS CHARACTERISTICS

FEBEX bentonite pellets
 Bentonite compacted at 1.36 g/cm^3 with $w=4.7\%$
 Bentonite height: 5/10 cm, diameter: 10/7 cm
 Deionised water injected on top at 0.15 / 2 bar



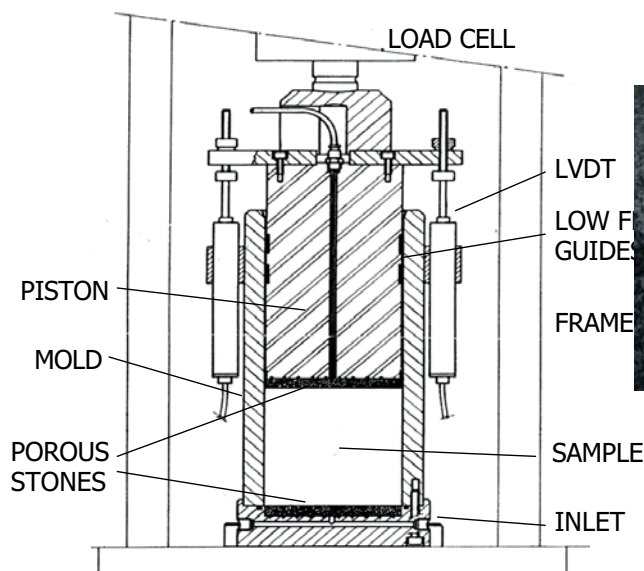
EB in situ test, Mont Terri

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Infiltration tests with FEBEX pellets: characteristics

On line measurement of swelling pressure, water intake and hydraulic conductivity
 Upon dismantling: determination of dry density, water content, basal spacings, porosity distribution, specific surface area

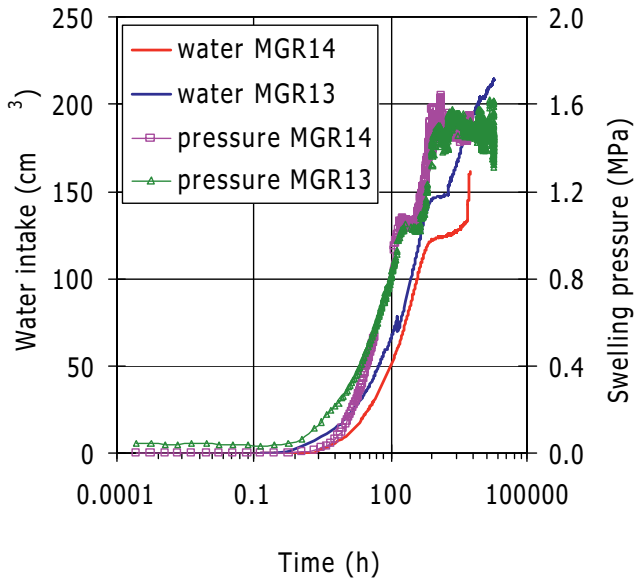


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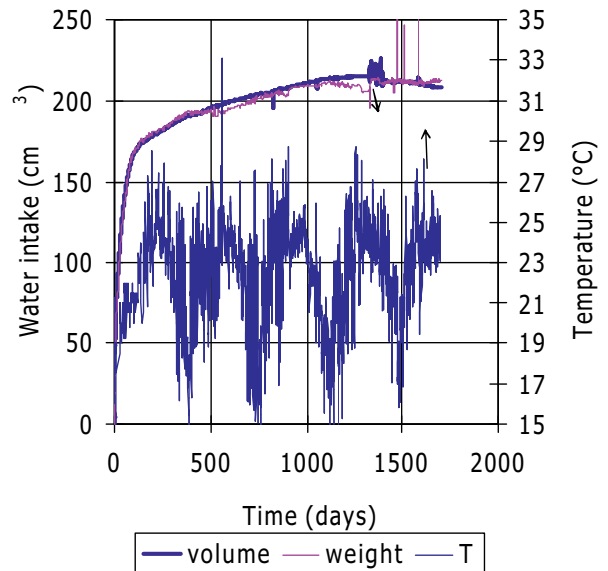
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Infiltration tests with FEBEX pellets: online results

MGR13: 1083 days; MGR14: 265 days
Height: 5 cm, diameter: 10 cm



INF_PELL1: 1703 days
Height: 10 cm, diameter: 7 cm



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Infiltration tests with FEBEX pellets: postmortem results



| | MGR13, 1083 days, P_s 1.49 MPa | | | | MGR14, 265 days, P_s 1.46 MPa | | | |
|----------|----------------------------------|-------------------------------------|-----------------|------------|---------------------------------|-------------------------------------|-----------------|------------|
| Position | Final w (%) | Final ρ_d (g/cm ³) | Final S_r (%) | $d(001)$ Å | Final w (%) | Final ρ_d (g/cm ³) | Final S_r (%) | $d(001)$ Å |
| Upper | 35.9 | 1.35 | 98 | 19.65 | 35.0 | 1.39 | 100 | 18.31 |
| Central | 35.8 | 1.36 | 99 | 19.57 | 35.6 | 1.38 | 100 | 18.50 |
| Bottom | 38.3 | 1.31 | 94 | 19.75 | 39.7 | 1.28 | 97 | 18.60 |
| Average | 36.7 | 1.34 | 97 | 19.66 | 36.8 | 1.35 | 99 | 18.47 |

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Infiltration tests with FEBEX pellets: postmortem results



BET surface area: 68 m²/g

t-plot μ pore volume: 0.01 cm³/g

| Position | Final w (%) | Final ρ_d (g/cm ³) | Final S_r (%) | $d(001)$ Å |
|----------|---------------|-------------------------------------|-----------------|------------|
| 1 | 40.1 | 1.30 | 100-106 | 19.03 |
| 2 | 38.7 | 1.34 | 103-106 | 17.91 |
| 3 | 38.6 | 1.33 | 101-106 | 18.46 |
| 4 | 38.9 | 1.32 | 101-106 | 18.51 |
| 5 | 38.8 | 1.34 | 103-106 | 18.51 |
| Average | 39.1 | 1.32 | 101-106 | 18.48 |

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Infiltration tests with FEBEX pellets: CONCLUSIONS

- ✓The increase/decrease/increase pattern of swelling pressure development appears irrespective of dry density, size of sample and fabric
- ✓The kinetics of the process and the P_s value depend on dry density and initial water content
- ✓The mixtures become homogeneous upon saturation, with P_s and k_w similar to those of compacted powder of the same dry density
- ✓Scale effect: P_s obtained in big oedometers tends to be higher
- ✓The basal spacing of the montmorillonite saturated and compacted at 1.4 g/cm³ corresponds to the 3-layer hydrate


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AIMS

- Evaluate the key HM processes and parameters taking place during the early evolution of the EBS
- Provide a reliable good quality experimental HM data base, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3

ACTIVITIES (all of them at lab T)

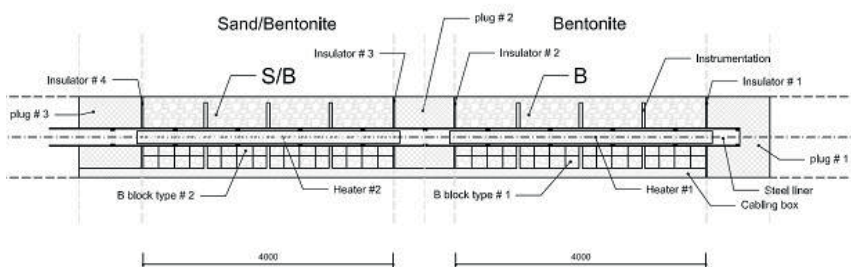
- Infiltration test with EB FEBEX pellets
- Infiltration tests with HE-E materials 
- Long-term infiltration tests with measurement of permeability at low hydraulic gradients (FEBEX and MX-80)

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Infiltration tests with HE-E materials

HE-E in situ test, Mont Terri



AIMS

- Provide support for the modelling of the **HE-E in situ test**
- Check the hydro-mechanical behaviour of the HE-E materials and compare it with that under thermal gradient
- Compare the HM behaviour of two different sealing materials

TESTS CHARACTERISTICS

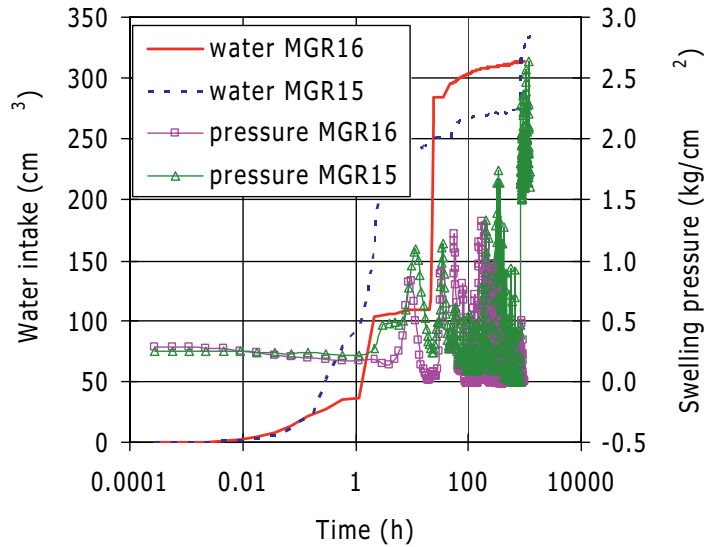
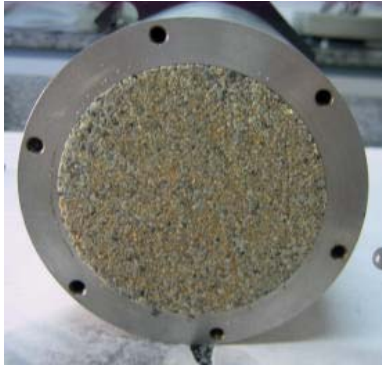
MX-80 bentonite pellets or sand/MX-80 mixture 65/35
 Initial in situ dry density and water content
 Sample height: 10 cm, diameter: 10 cm
 Pearson water injected on top at 0.14/2 bar

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Infiltration tests with HE-E mixture: online results

Sand/bentonite 65/35 mixture compacted at 1.46 g/cm^3 with $w=3\%$
 Test MGR15: Duration 51 days, final $w= 29.9\%$, final $S_r=96\%$
 Test MGR16: Duration 41 days, final $w=27.8\%$, final $S_r=88\%$



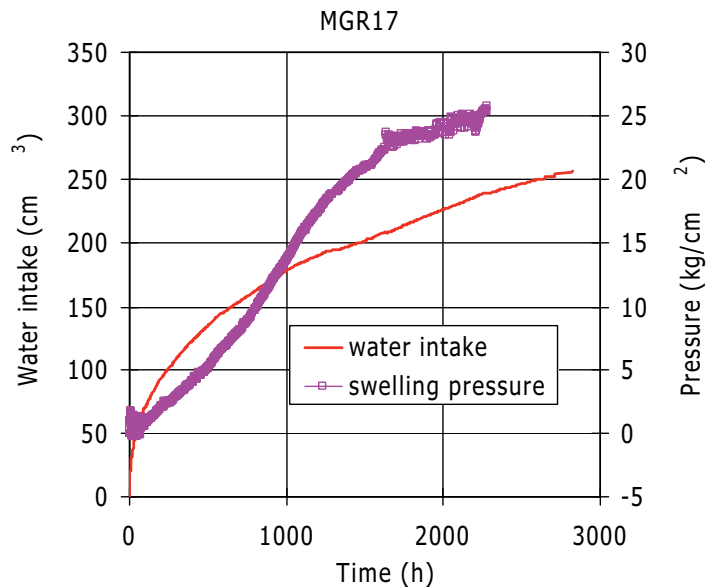
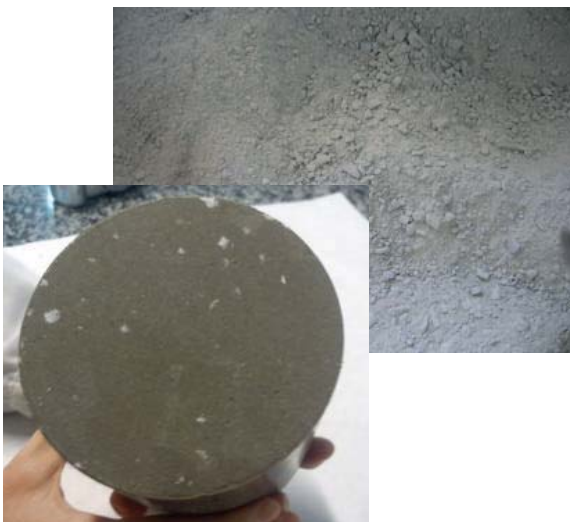
P_s measured in oedometer 0.1 MPa
 High hydraulic conductivity

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Infiltration tests with HE-E MX-80 pellets: online results

MX-80 pellets compacted at 1.47 g/cm^3 with $w=6.3\%$
 Test MGR17: Duration 118 days, final $w= 28.4\%$, final $S_r=98\%$
 Test MGR18: Duration >62 days



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AIMS

- Evaluate the key HM processes and parameters taking place during the early evolution of the EBS
- Provide a reliable good quality experimental HM data base, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3

ACTIVITIES (all of them at lab T)

- Infiltration test with EB FEBEX pellets
- Infiltration tests with HE-E materials
- Long-term infiltration tests with measurement of permeability at low hydraulic gradients (FEBEX and MX-80) ←

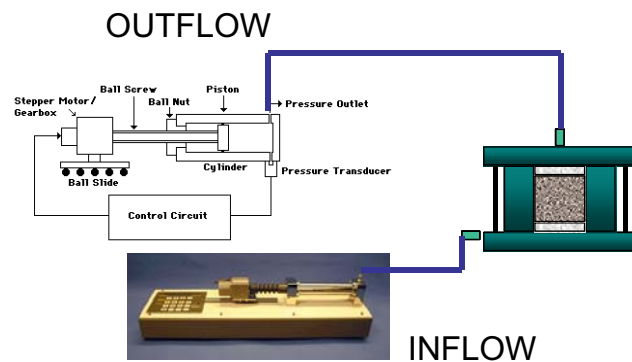
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Long term infiltration tests with measurement of permeability

TESTS CHARACTERISTICS

FEBEX and MX-80 bentonites compacted with hygroscopic water content at dry densities 1.4-1.7 g/cm³
 Bentonite height: 2.5 cm, diameter: 5 cm
 Saturation with deionised water injected at 6 bar
 Measurement of permeability applying hydraulic gradients between 200 and 7500



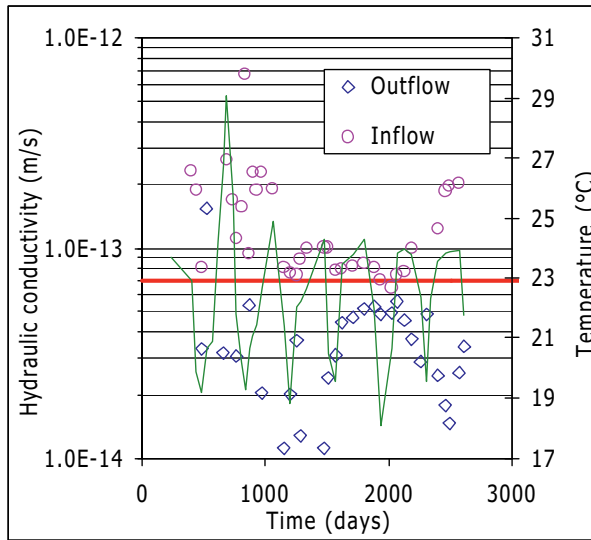
AIMS

- Check the possible evolution of permeability over time
- Check the range of validity of Darcy's law
- Check the effect of hydraulic gradient on flow (existence of a threshold gradient)
- Provide information about the changes of adsorbed water density

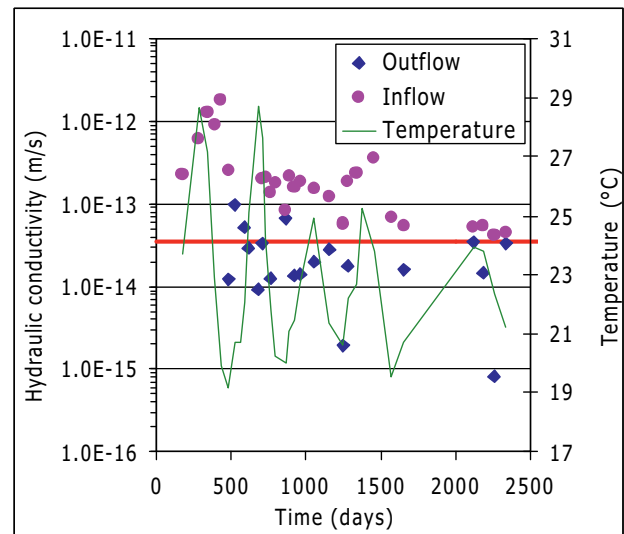
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Long term infiltration tests with measurement of permeability: FEBEX bentonite



$\rho_d = 1.55 \text{ g/cm}^3$



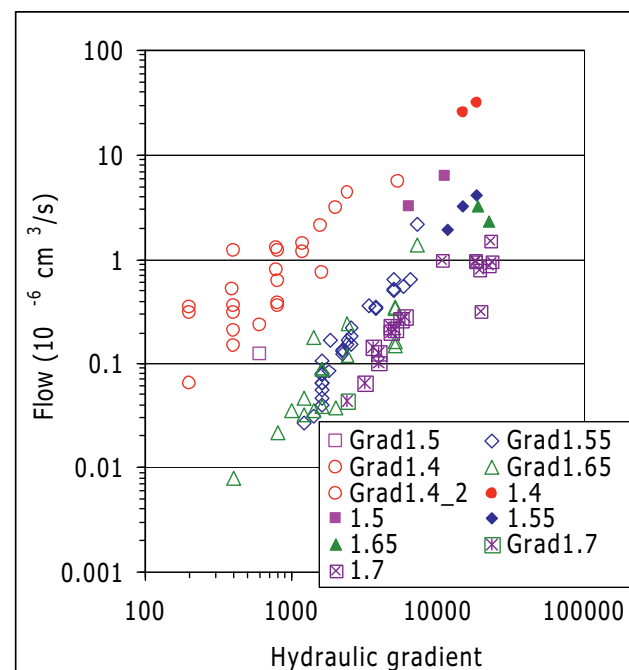
$\rho_d = 1.65 \text{ g/cm}^3$

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Long term infiltration tests with measurement of permeability: FEBEX bentonite

- No clear evolution of permeability with time was observed for more than 2300 days
- Inflow continues to be smaller than outflow after 2300 days: it is coming in more water than is getting out
- Possible critical gradient around 2000 and threshold gradient between 200 and 1400 depending on dry density and injection pressures
- Above these gradients, the validity of Darcy's law was checked



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- T21. EXPERIMENTATION ON KEY HM PROCESSES AND PARAMETERS (in situ and laboratory)
- **T221. LABORATORY EXPERIMENTATION ON KEY THM PROCESSES AND PARAMETERS (mock-up and laboratory)** 
- T231. THM-C MOCK-UPS (GAME TESTS)
- T232. THM AND THMC TESTS AIMED AT THE UNDERSTANDING OF KEY PROCESSES TAKING PLACE AT THE INTERFACES (laboratory)

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T221. LABORATORY EXPERIMENTATION ON KEY THM PROCESSES AND PARAMETERS

AIMS

- Evaluate the key THM processes and parameters taking place during the early evolution of the EBS
- Provide a reliable good quality experimental THM data base, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3

ACTIVITIES

- The FEBEX mock-up: operation and sampling book 
- Long-term THM tests in cells simulating particular disposal concepts
 - Tests already running
 - New tests

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FEBEX mock-up test

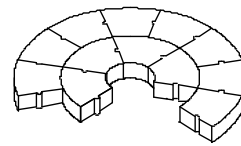
AIMS

- Evaluation of the performance of the instruments and monitoring system
- Verification of some hypothesis on the THM processes in the transient phase of the barrier material



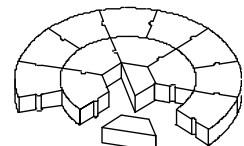
TESTS CHARACTERISTICS

Thickness of FEBEX bentonite barrier: 63 cm
 Barrier dry density: 1.65 g/cm³ (22300 kg of bentonite)
 Duration: ongoing for 15 years
 Data provided: online measurements
 Particularities: initial injection of 634L (w=17.1%), overheating episodes



Section with heater

98±2°C

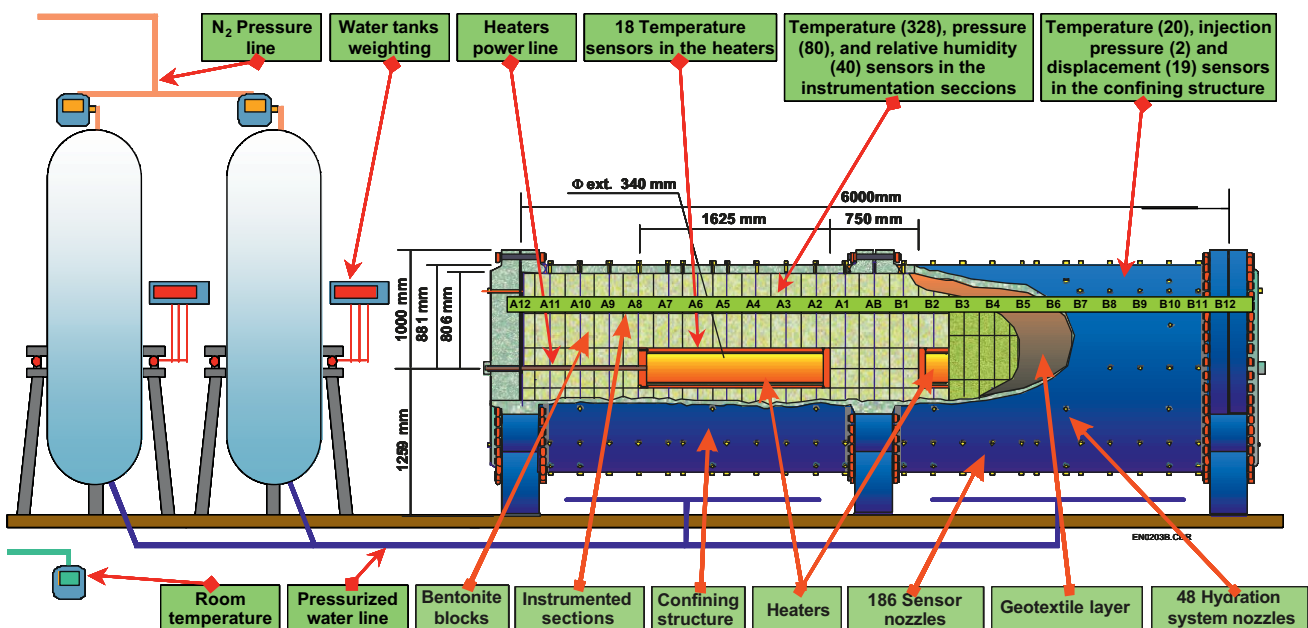


Section without heater

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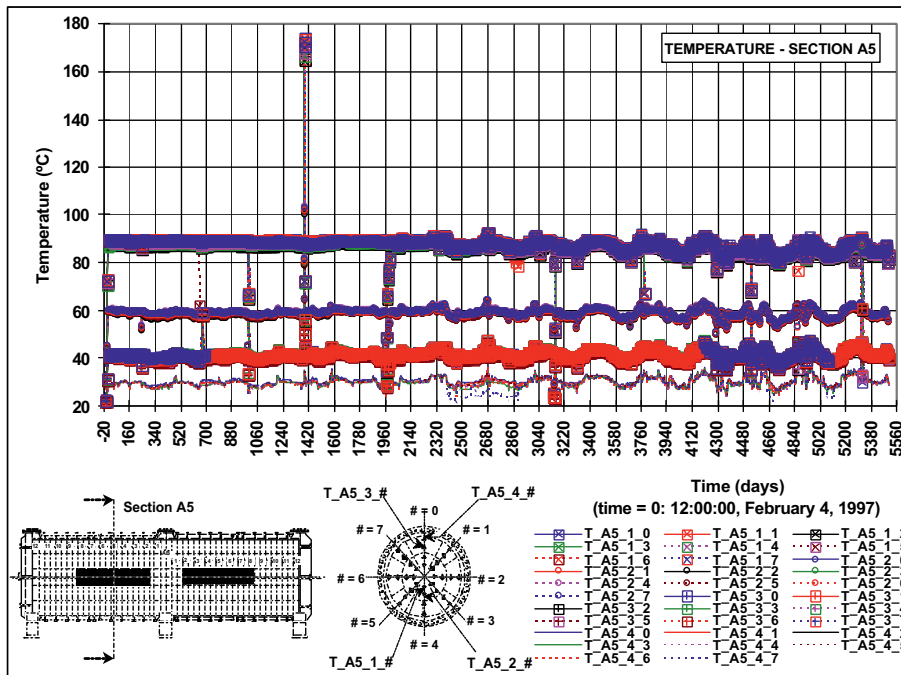
FEBEX mock-up test: configuration



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FEBEX mock-up: temperature



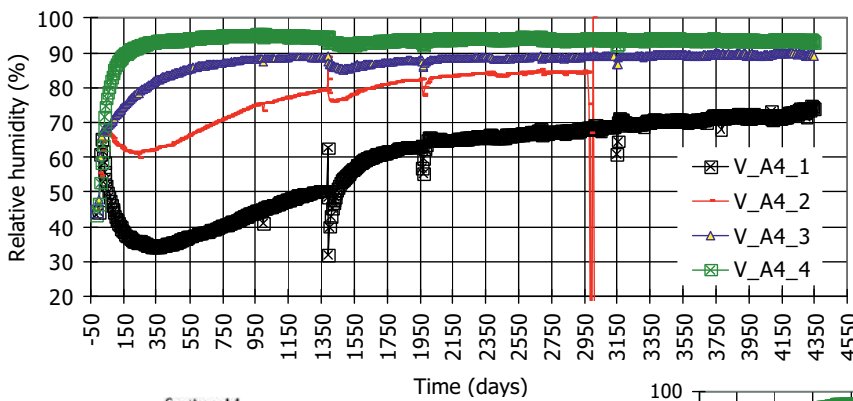
Seasonal changes due to the constant power supply (from day 2300, 2700 W/heater)

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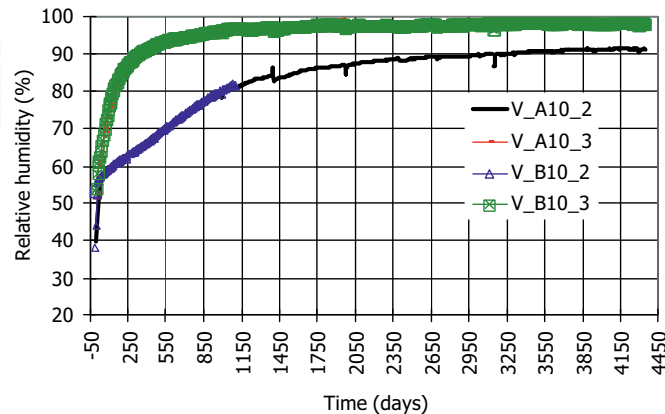


FEBEX mock-up: relative humidity



Hot zones: from 74 to 85% RH (~ 49 to 27 MPa at 80°C).

Cold zones: maximum variation is lower than 2% RH (~ 3 MPa at 30°C).

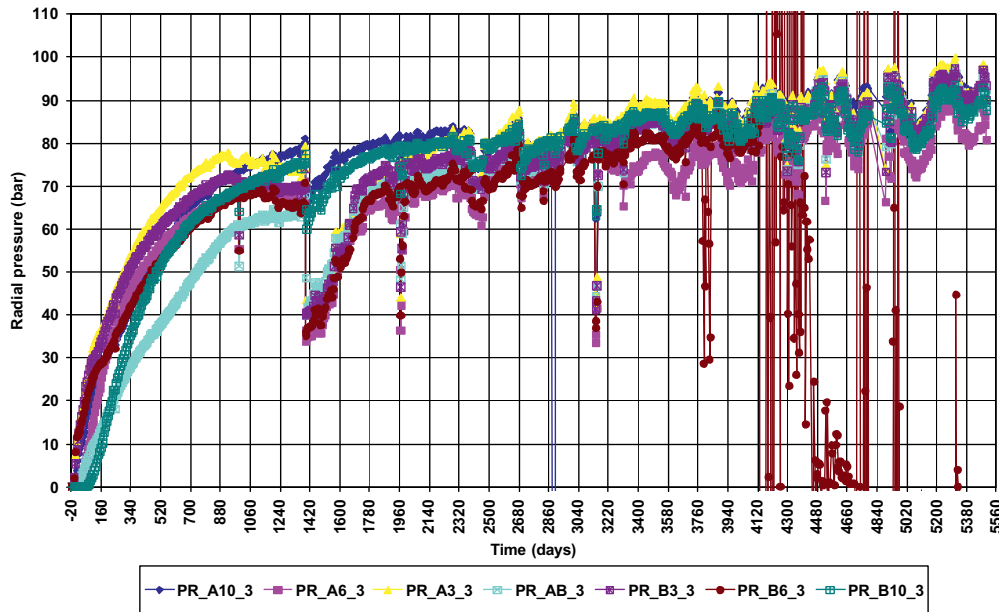


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FEBEX mock-up: pressure



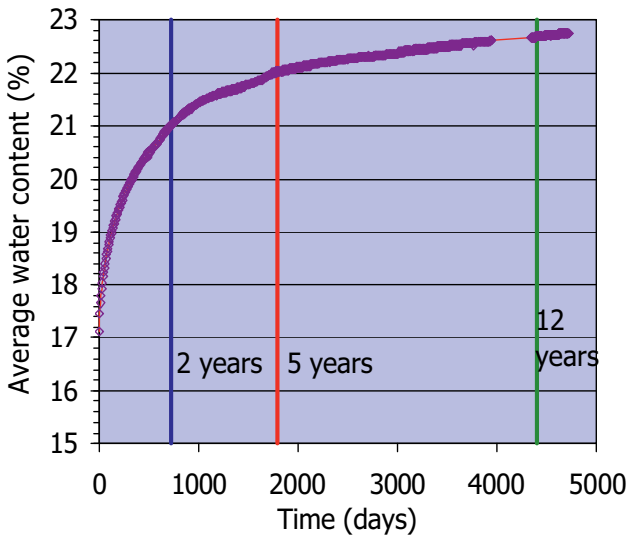
The pressure range is reduced as the external zone of the barrier becomes saturated and the local heterogeneities disappear (radial pressure: 8-10 MPa, higher in the outer ring). Pressure-temperature coupling.

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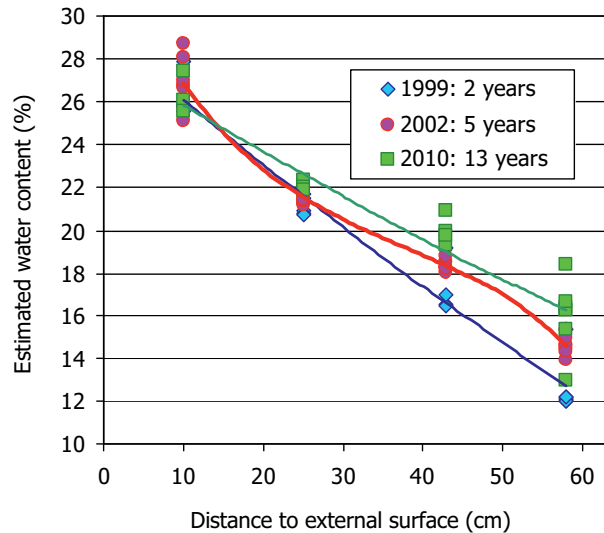
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FEBEX mock-up test: water content

Water content computed from measured water intake



Water content around heaters inferred from RH measurements and WRC



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FEBEX mock-up test: sampling book

LOCATION
"As built" x coordinate -1.250
Bentonite slice 10B
Instrumented section B5

SAMPLING SECTION 10B

| SAMPLES | | | | | | |
|---------|----------------|-----------|-------|--------------------|----------------|---------|
| Code | No. of samples | Type | Shape | Sampling procedure | Dimension (mm) | Partner |
| | 5 + 5 | Bentonite | Core | | | CIEMAT |
| | 1 | Bentonite | Core | | | CIEMAT |
| | 5 | Bentonite | Block | | | CIEMAT |
| | 1 | Bentonite | Block | | | CIEMAT |
| | 5 | Bentonite | Core | | | CIEMAT |
| | 1 | Bentonite | Block | | | CIEMAT |
| | 5 | Bentonite | Core | | | CIEMAT |
| | 1 | Bentonite | Block | | | CIEMAT |
| | 5 | Bentonite | Core | | | CIEMAT |
| | 2 | Metal | Rack | | | CIEMAT |

| INSTRUMENTS | | | | | | |
|-------------|----------------|-------------------|---------|-------------|-----------|--|
| Code | No. of sensors | Type of Measure | Partner | Comments | | |
| T_BS_#_0 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |
| T_BS_#_1 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |
| T_BS_#_2 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |
| T_BS_#_3 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |
| T_BS_#_4 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |
| T_BS_#_5 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |
| T_BS_#_6 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |
| T_BS_#_7 | 4 | Pt100 temperature | CIEMAT | Calibration | Corrosion | |

INSTALLATION PHOTO

Figure 1: "As built" bentonite section 10B.

LOCATION
"As built" x coordinate -1.250
Bentonite slice 10B
Instrumented section B5

SAMPLING SECTION 10B

Figure 1: Location of sampling section 10B.

Figure 2: Sampling section 10B. Instrumented section 6B. Tracer section

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FEBEX mock-up test: CONCLUSIONS

Data base:

Monitoring of the behaviour of the Mock-up provides a long-term data base (up to 15 years) on the evolution of the thermal, hydraulic and mechanical parameters of the clay barrier.

THM parameters measurement:

Evaluation of the performance and long-term behaviour of the THM monitoring systems.

THMC numerical models:

Improvement of models with current THM information, in addition to the final picture after dismantling.

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AIMS

- Evaluate the key THM processes and parameters taking place during the early evolution of the EBS
- Provide a reliable good quality experimental THM data base, including different time and spatial scales, as input to the modelling and extrapolation work to be conducted within WP3

ACTIVITIES

- The FEBEX mock-up (operation and sampling book)
- Long-term THM tests in cells simulating particular disposal concepts
 - Tests already running
 - New tests



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THM tests in cells: FEBEX, 40 cm long

AIMS

- Check the long-term evolution of saturation
- Check the influence of thermal gradient on saturation

TESTS CHARACTERISTICS

Material: FEBEX bentonite
 Height of bentonite column: 40 cm
 Initial dry density and water content: 1.65 g/cm³, 13.1%
 Duration: ongoing for 10 years
 Hydration: granitic water, 1 MPa
 Heater T bottom: 100°C (GT), amb (I)
 Upper T: room
 Data provided: RH and T online, information about THMG changes upon dismantling

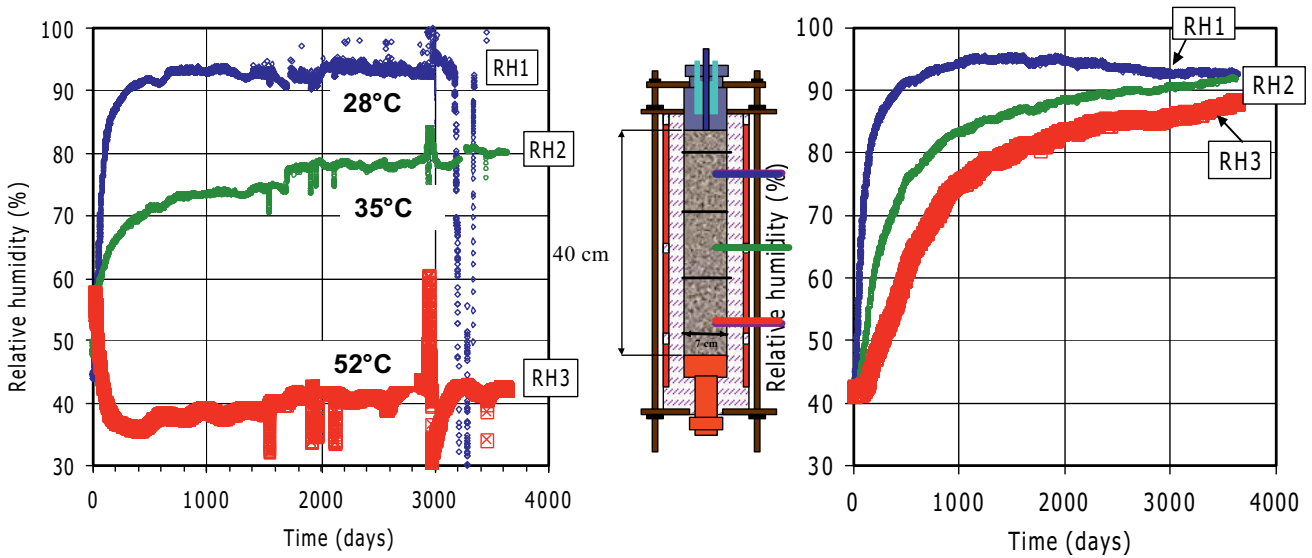


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THM tests in cells: FEBEX, 40 cm long

Online relative humidity measurements



Test under thermal gradient (heater T: 100°C)

Isothermal test, room T

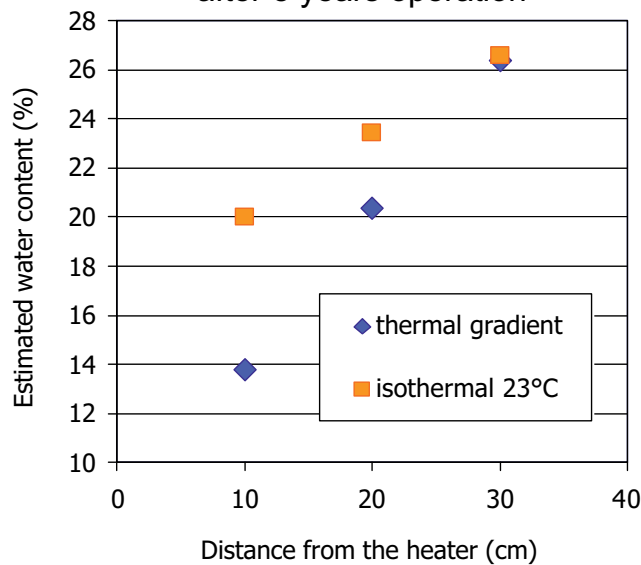
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THM tests in cells: FEBEX, 40 cm long

Inferred water content from RH measurements and WRC after 8 years operation



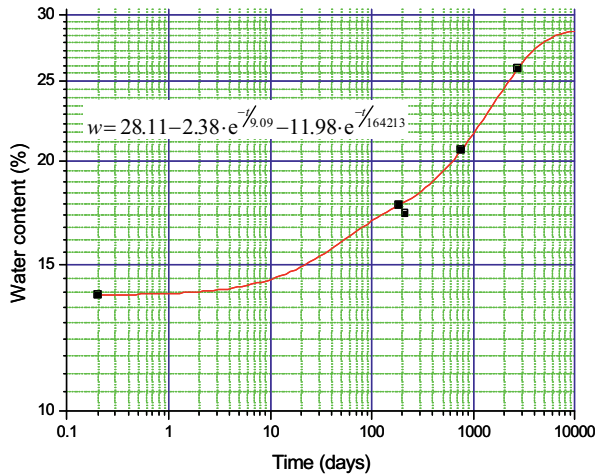
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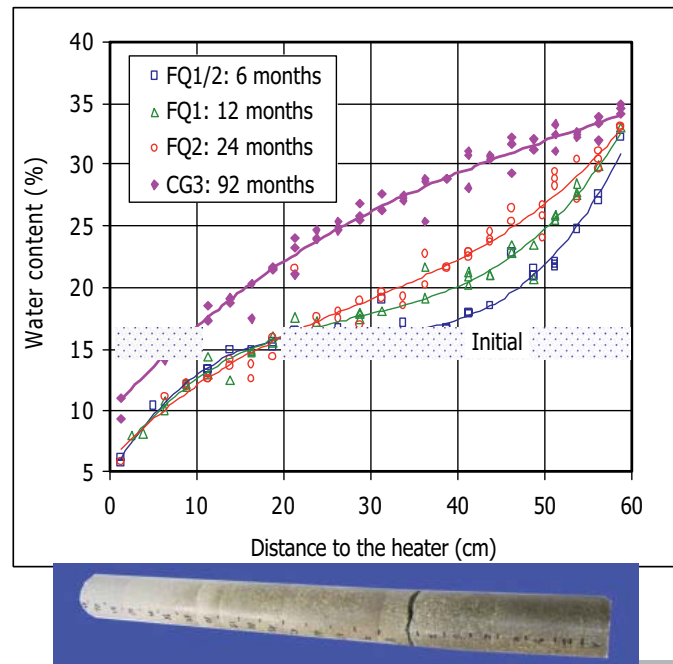


THM tests in cells: previous experience in 60-cm long cells

Measured final average water content



Final measured water content distribution



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THM tests in cells: CONCLUSIONS

- Water vapour moved very quickly, causing local water content increases, while thermal gradient delayed saturation in the inner barrier.
- Water content and density gradients were generated in the bentonite during the transient period of saturation.
- Once the barrier becomes saturated the average density of the water adsorbed in smectite will be higher than 1 g/cm^3 .
- The water movement, both in liquid and vapour phase, results in geochemical modifications, particularly of the pore water composition, that can also influence the barrier behaviour.
- The rate of hydration of the barrier depends on bentonite and surrounding media permeabilities, waste temperature and buffer thickness and geometry.

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THM tests in cells: HE-E materials

AIMS

- Provide support for the modelling of the HE-E in situ test
- Check the behaviour of barrier materials at $T > 140^\circ\text{C}$

TESTS CHARACTERISTICS

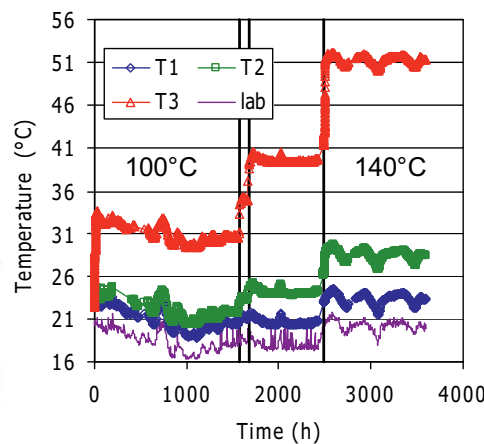
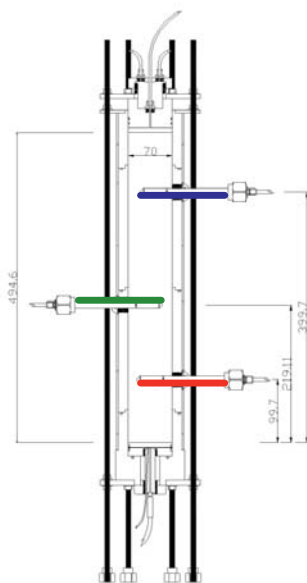
Material: HE-E sand/bentonite (65/35) mixture, MX-80 pellets
 Height of column: 50 cm
 Initial dry density and water content: 1.45 g/cm^3 and 3.6%, 1.52 g/cm^3 and 6.4%
 Heater T bottom: 100°C – 140°C
 Upper T: room
 Hydration: Pearson water, no P
 Data provided: online measurements of RH, T, water intake, heater power



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THM tests in cells: HE-E sand/bentonite mixture

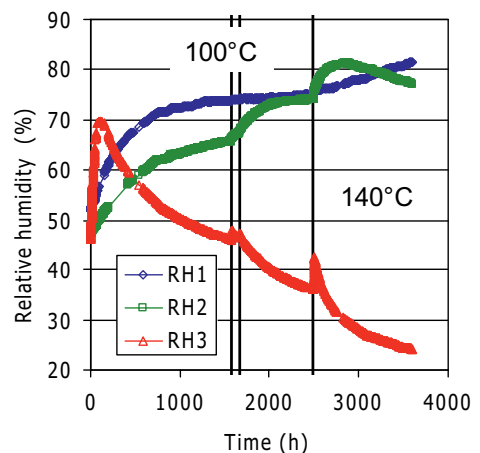


Quick thermal steady state

Low temperatures in the material due to its low thermal conductivity and heat losses

Quick movement of the vapour phase towards cooler areas

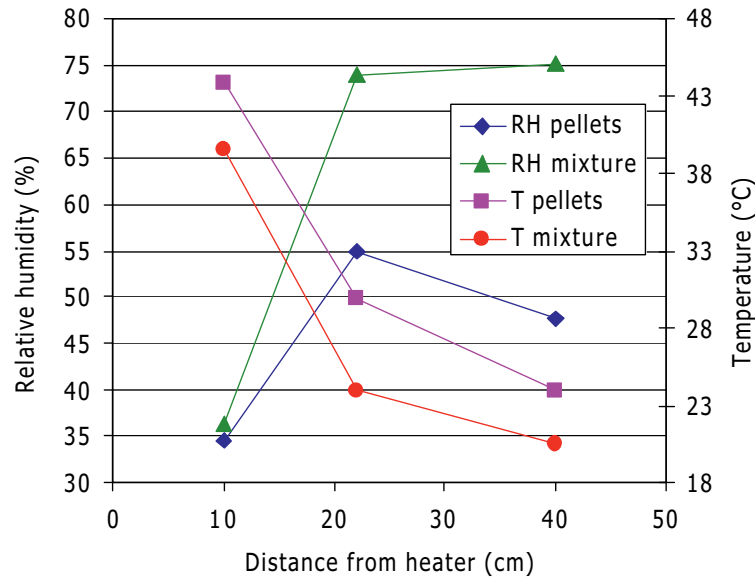
Much longer time for hydraulic steady state



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THM tests in cells: HE-E materials



Steady values for a heater temperature of 100°C

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Tasks

- T21. EXPERIMENTATION ON KEY HM PROCESSES AND PARAMETERS (in situ and laboratory)
- T221. LABORATORY EXPERIMENTATION ON KEY THM PROCESSES AND PARAMETERS (mock-up and laboratory)
- **T231. THM-C MOCK-UPS (GAME TESTS)** ←
- T232. THM AND THMC TESTS AIMED AT THE UNDERSTANDING OF KEY PROCESSES TAKING PLACE AT THE INTERFACES (laboratory)

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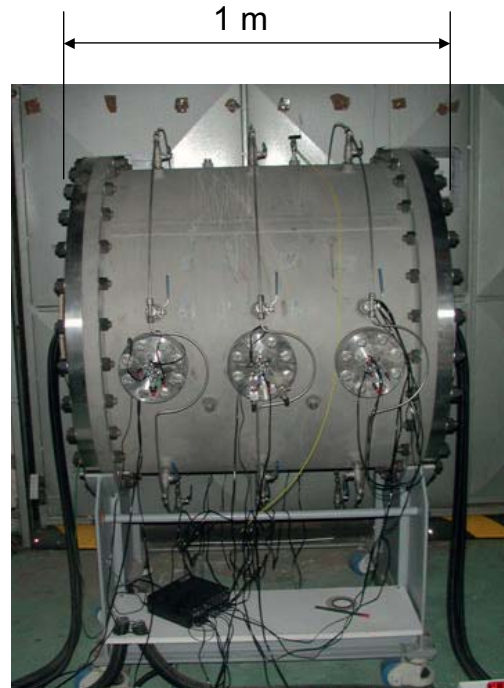


AIMS

- Investigate the changes that may occur in the key parameters of the buffer material as a result of THM and THC processes
- Investigate the geochemical changes by sampling of pore water, if available, with the minimum possible interference with the system

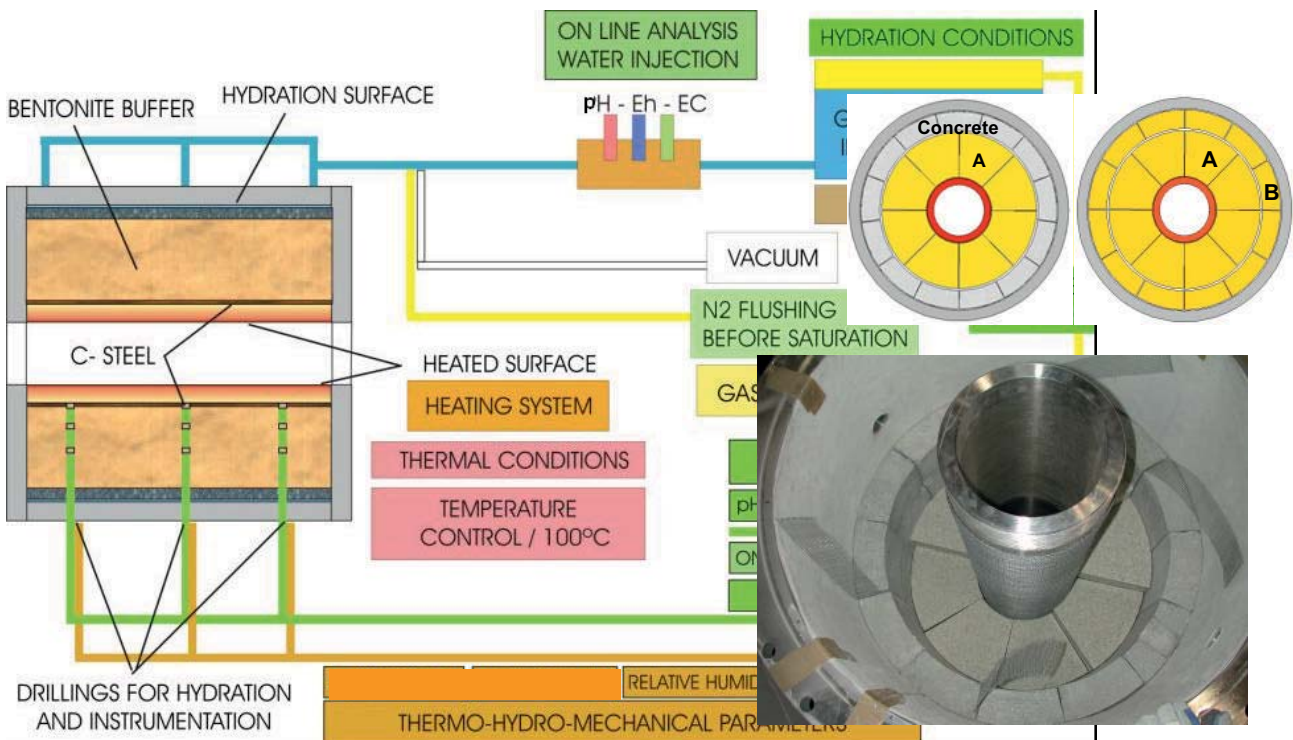
TESTS CHARACTERISTICS

Material: FEBEX bentonite / FEBEX and concrete
 Thickness of barrier: 30 cm / 22 cm
 Initial dry density and water content: 1.6 g/cm³, 14%
 Duration: ongoing for 7 years, with interruptions
 Hydration: granitic water / synthetic saline water
 Heater T: maximum 40°C
 Data provided: bentonite RH and T, water intake, water pH and conductivity, heater power and T



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Outer ring

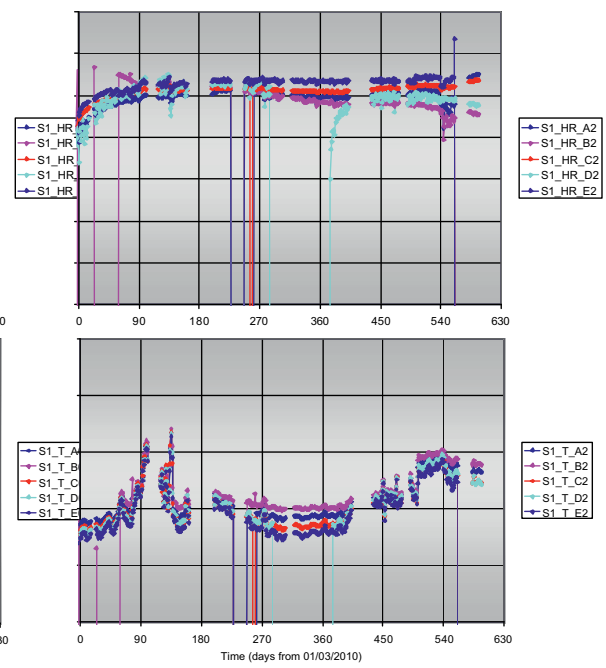
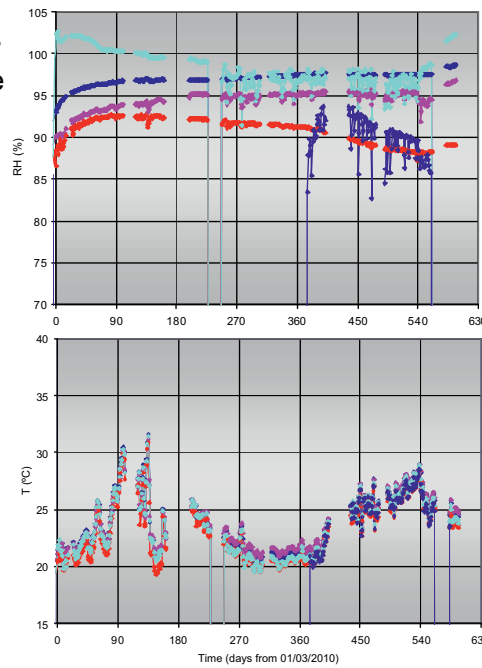
Inner ring

Most RH values
in both tests are
>90%

Many sensors
damaged and
replaced

Corrosion
processes are
taking place

Main outcome
will be upon
dismantling



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Tasks

- T21. EXPERIMENTATION ON KEY HM PROCESSES AND PARAMETERS (in situ and laboratory)
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- T231. THM-C MOCK-UPS (GAME TESTS)
- **T232. THM AND THMC TESTS AIMED AT THE UNDERSTANDING OF KEY PROCESSES TAKING PLACE AT THE INTERFACES (laboratory)** ←

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AIMS

- Understand the key processes taking place at the interfaces (canister-bentonite-concrete)
- Investigate the sequence of corrosion/alteration products and processes at the canister-bentonite-concrete interface under conditions as close as possible to those of the repository
- Investigate how these processes affect the properties of the bentonite

TESTS CHARACTERISTICS

Material: FEBEX bentonite / concrete / corrosion products

Initial dry density and water content: 1.65 g/cm³, 14%

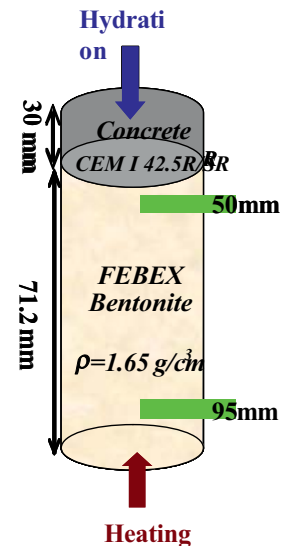
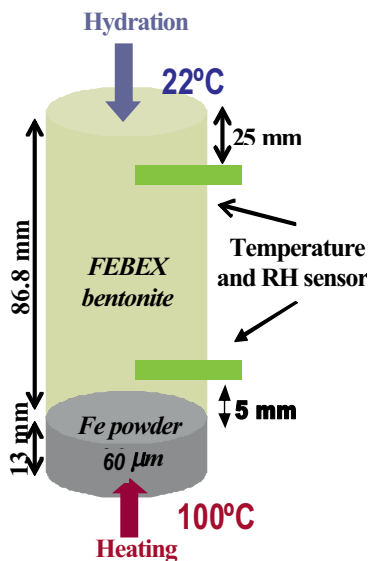
- Intermediate cells: heater T 100°C, thickness of bentonite 7-9 cm, duration from 0.5 to 7 years, granitic water GTS / synthetic saline water
- Small cells: isothermal at 60°C, thickness of bentonite 1.8 cm, duration 18 months, saline hydration water



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Experiments representative of corrosion/alteration under unsaturated conditions – **Post-closure-transient state**
Started during NF-PRO – Going on in PEBS

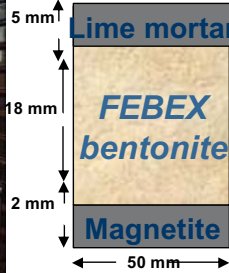


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Experiments representative of corrosion/alteration under saturated conditions – **Transient-saturated state**

Started during NF-PRO (with C-steel plates and iron powder) –
Going on in PEBS



Temp: 60°C

Magnetite as final canister corrosion product

Lime mortar as concrete degradation product

Start 15/03/2011

Foreseen end 15/09/2012

Total: 18 months

April, 25th and 26th 2012

Regulatory Authority Workshc

Canister/bentonite interface

Evolution of corrosion products with time

- FeOOH (Fe^{3+}) **6 months** Aerobic conditions
- Fe_2O_3 (Fe^{3+}) **15 months** Aerobic to suboxic
- $\text{Fe}(\text{OH})_2/\text{Fe}_3\text{O}_4$ (Fe^{2+}) **52 months** Suboxic conditions

| Fe powder | | |
|---------------|---------------|---------------|
| 6 months | 15 months | 52 months |
| | | |
| February 2007 | November 2008 | December 2010 |

Fe powder: slight corrosion

- *Non-corroded areas* (metallic luster): no chlorides
- *Corroded areas*
 - traces of chlorine and calcium
 - cracks in the oxide layer

Presence of Cl in corrosion products

April, 25th and 26th 2012

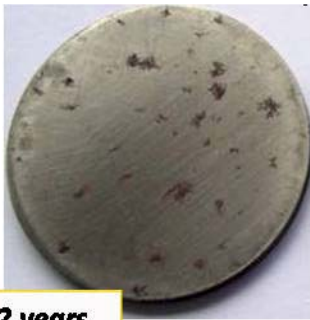
Regulatory Authority Workshc

Canister/bentonite interface

Results on carbon steel plates – Corrosion Rates

Unsaturated conditions

Heater T: 100°C



2 years

Droplets of water by deliquescence of salts (**chlorides**)
Initialization of localised corrosion whilst bentonite is not fully saturated

Saturated conditions

Homogenisation of corrosion



Corrosion products



Clean surface

Corrosion rate after 2 years:

2.1 µm/y

In good agreement with previous studies

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Regulatory Authority Workshc

Canister/bentonite interface

No mineralogical alteration of bentonite at the steel/bentonite interface

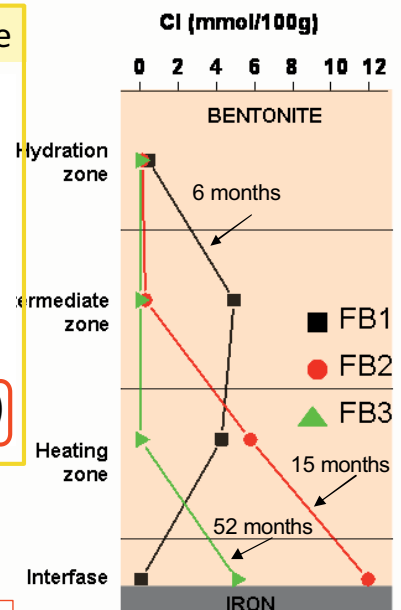
Geochemical processes observed in compacted bentonite

Simultaneous hydration and heating causes:

- **Dissolution and dilution** of more soluble accessory minerals (*chlorides, sulfates and carbonates*)
- **Advection** as the predominant process for ion movement: *unsaturated state*
- **Generation of saline fronts (chloride, sulfate)**

Jeopardize the performance of the canister

Chloride can initialize **localized corrosion** during transient state



Chloride distribution

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Bentonite (FEBEX) /concrete (CEM I, SR-type) interface

Background: ECOCLAY PROJECTS, NFPRO

Alkaline waters from the concrete will diffuse through the clay barrier. The high pH (12.5 to 13.4) of the pore waters of concrete contrasts with the pH (7 to 8) of the pore waters in bentonite:

pH > 13: **high reactivity**; montmorillonite dissolution, precipitation of zeolites (phillipsite-analcime), Mg- tri-octahedral sheetsilicates, CSH gels and brucite

pH < 13: **low reactivity**; (portlandite solubility equilibrium): prevalence of precipitation of CSH and dissolution/precipitation of carbonates

Development of alkaline reaction front through bentonite

(up to 1.5 years experiments) :

Mineralogical alteration < 5 mm

Geochemical alteration (cation exchange, slow rate dissolution/ precipitation processes (>> 2 cm; depends on test size and sensibility of determinations)

April, 25th and 26th 2012

Regulatory Authority Workshc

Bentonite (FEBEX) /concrete (CEM I, SR-type) interface

PEBS PROJECT

Previous studies focused mainly on a highly reactive alteration environment (pH>13) at short-term.

PEBS: Concrete-compacted bentonite interaction studied containing the materials and **conditions as close as possible to real ones**, with simultaneous heating and hydration at **long-term** (continued from NF-Pro CIEMAT tests).

Development of alkaline reaction front through bentonite

(up to 4.5 years experiments) :

Mineralogical alteration: Calcite, aragonite, and CSH/CASH compounds varying Ca/Si ratios (0.5-1.5) developed in < **1.5 mm** thickness.

Geochemical alteration: Cation exchange (Ca,Na increase , Mg decrease) > **3 cm**, affected by the opposite heat source also.

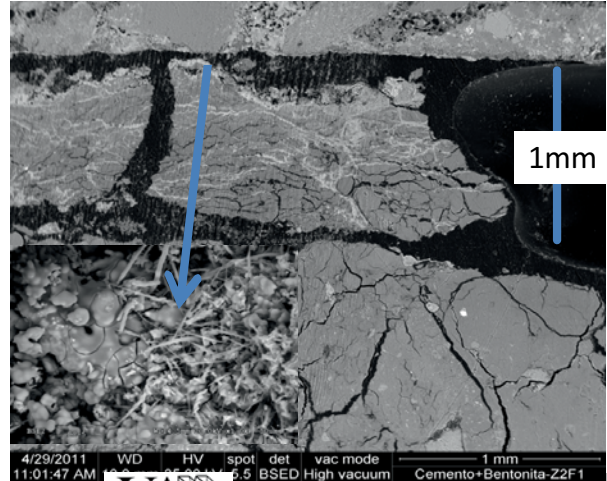
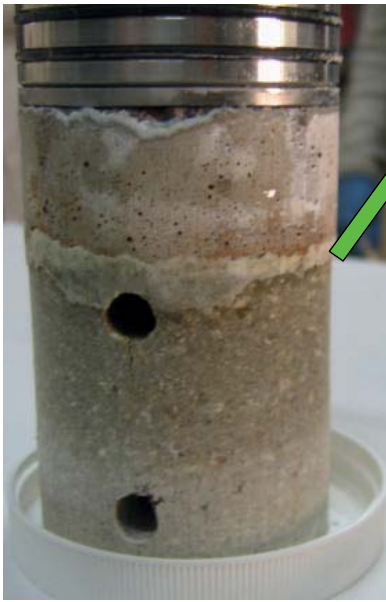
Ongoing research: Nature of CSH CASH phases / impact on THM properties

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Regulatory Authority Workshc

Bentonite (FEBEX) /concrete (CEM I, SR-type) interface

4.5-year long test in intermediate cell



Mineralogical transformations:
carbonates and CASH Ca/Si 0.5-1.5

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Regulatory Authority Workshc

The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 249681

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April, 25th and 26th 2012

Regulatory Authority Workshop

PEBS – Long Term Performance of Engineered Barrier systems

HE-E experiment in the VE Test Section

EBS behaviour immediately after repository closure in a clay host rock

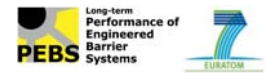
Irina Gaus

Klaus Wiczorek, Kristof Schuster, Juan Carlos Mayor, Paul Marschall, Patrick Steiner, Thomas Trick, Ursula Rösli, José-Luis García Siñeriz, Christophe Nussbaum, Oliver Czaikowski, Uli Kuhlmann, Benoit Garitte, Antonio Gens, Manuel Velasco, Sven Köhler, Sven-Peter Teodori, Hanspeter Weber

Workshop for Regulatory Authorities 26 April 2012 – Mont Terri



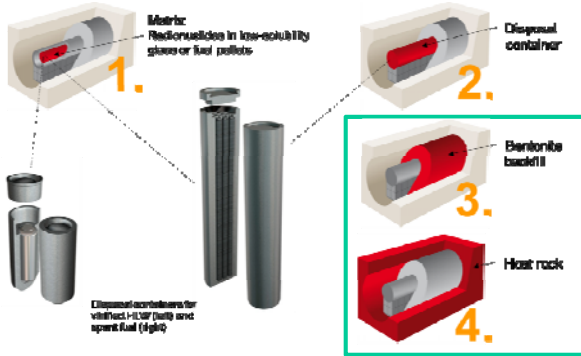
Outline of this presentation



- Introduction to the experiment
- Construction of the experiment (Jan-June '11)
- Ongoing monitoring since June 2011
- Modelling strategy and first results
- Conclusions so far

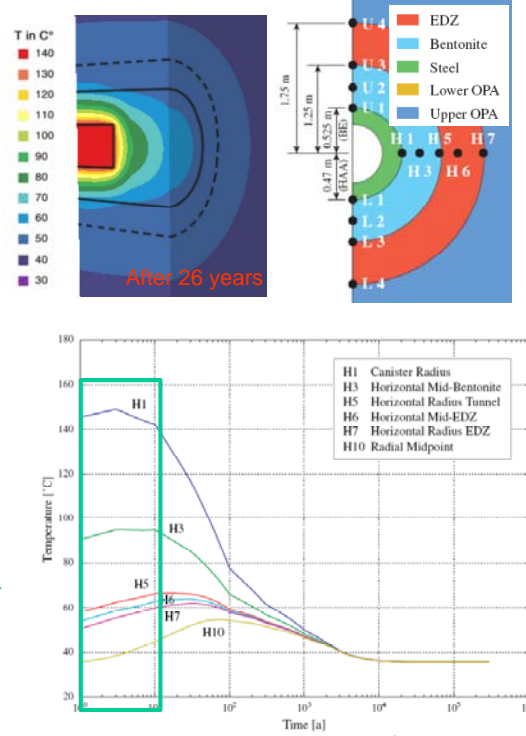
Background for this presentation

Disposal concept HLW and spent fuel



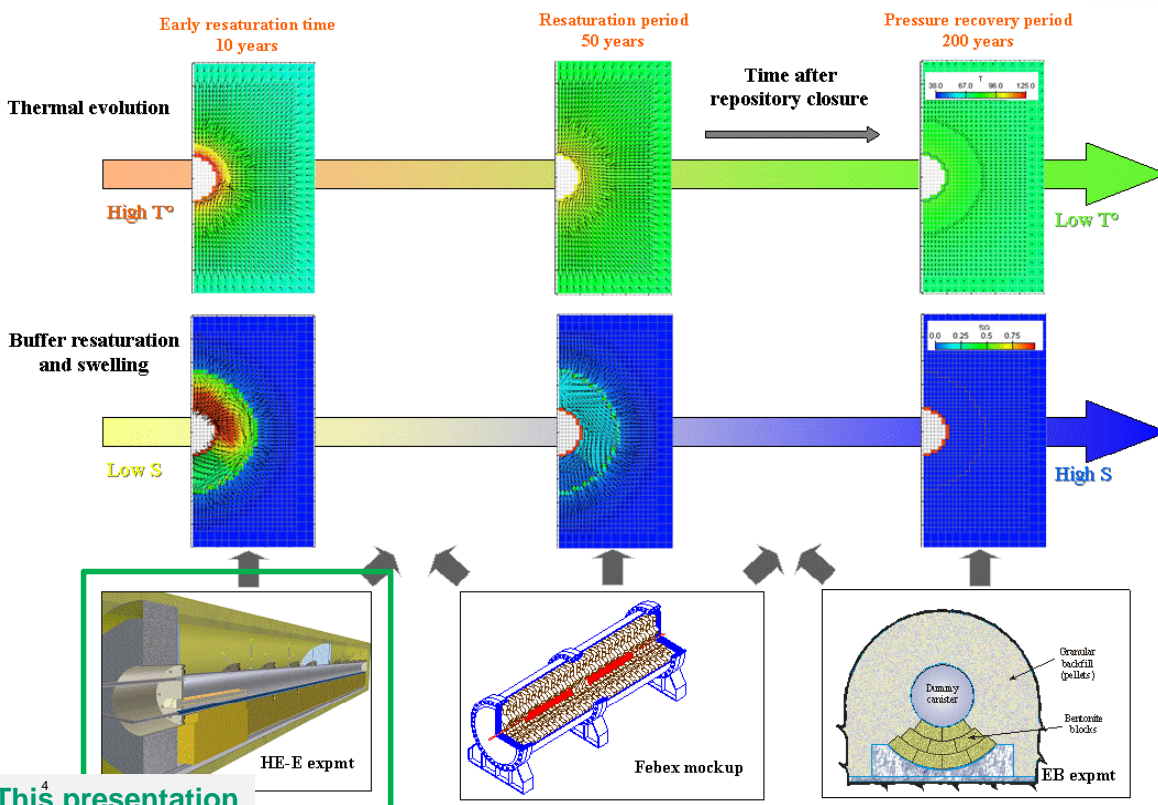
EBS and host rock evolution at initial high T°

Modelled heat transmission in HLW tunnels



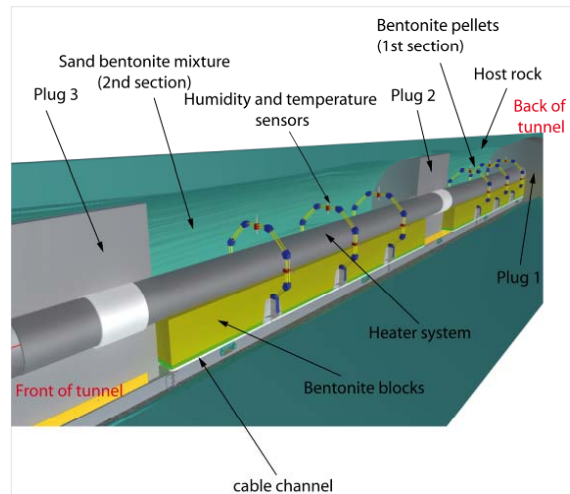
(Johnson et al., 2002)

Objectives of the PEBS project (2010-2014)



Objectives of the HE-E heater experiment

- Elucidating the early non-isothermal resaturation period and its impact on the thermo-hydro-mechanical behaviour.
 - provide the **experimental data base** required for the calibration and **validation of existing thermo-hydraulic models** of the early resaturation phase
 - **upscale thermal conductivity** of the partially saturated buffer from laboratory to field scale:
 - pure bentonite
 - bentonite-sand mixture



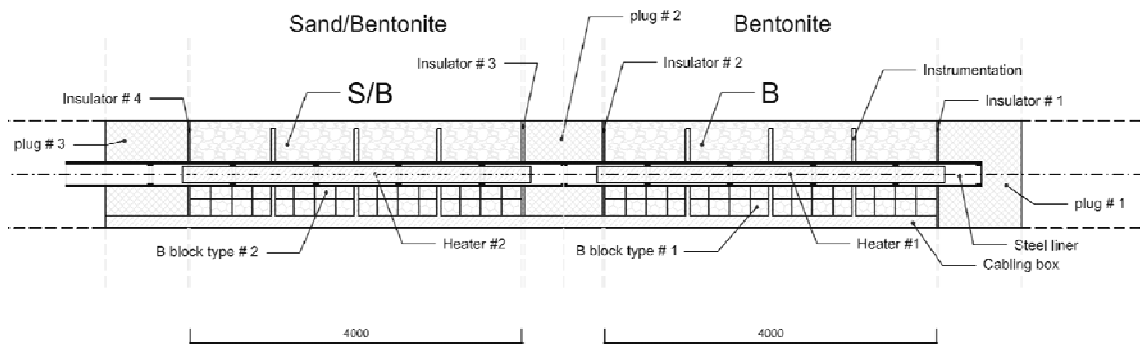
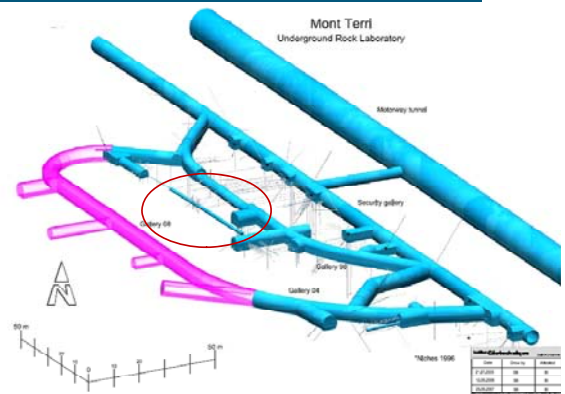
5

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HE-E heater experiment: characteristics

- 1:2 scale (microtunnel 1.3 m)
- Natural resaturation from clay hostrock
- Heater surface temperature: **140°C**
- Duration: June 2011 - >2014
- Two symmetrical sections - different granular materials



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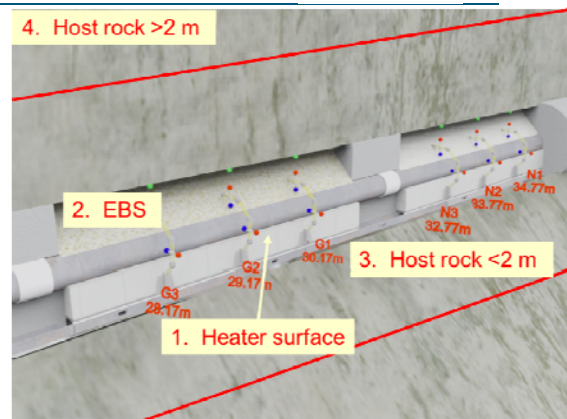
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Outline of this presentation

- Introduction to the experiment
- **Construction and start of the experiment**
- Ongoing monitoring since June 2011
- Modelling strategy and results
- Conclusions so far

Instrumentation concept – 4 areas

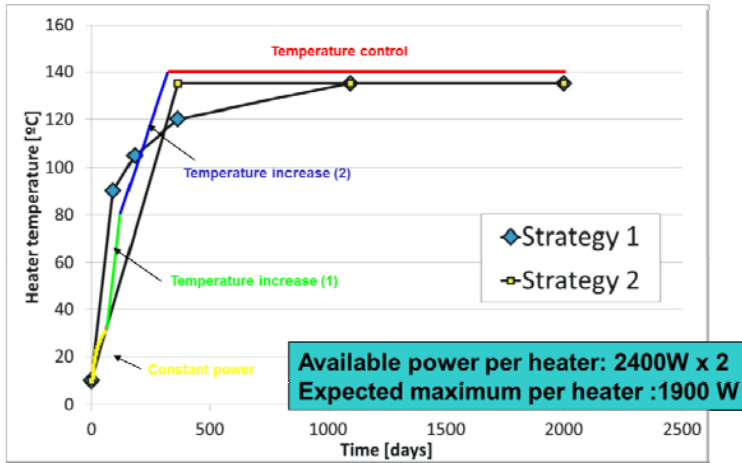
1. **Heater surface** → T° and applied power
2. **Engineered barrier** → T° and humidity
 - Heat transmission
 - Evaporation and condensation
3. **Opalinus clay close to microtunnel < 2 m**
 - T° , humidity, hydraulic pressure, displacement
 - Heat transmission
 - Partly desaturation
 - Pressure increases
 - Stress development
4. **The Opalinus clay > 2 m from microtunnel**
 - hydraulic pressure, T°
 - Heat transmission
 - Pressure increases



Indirect measurements:

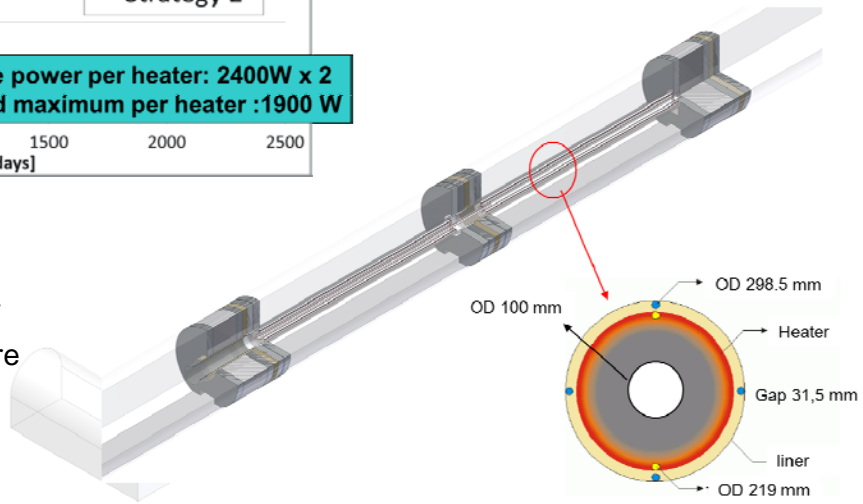
- **Seismics:** array with 5 emitting and 10 receiving transducers
- **Geoelectric:** electrode array in 1 m deep boreholes

Heater system – heating strategy

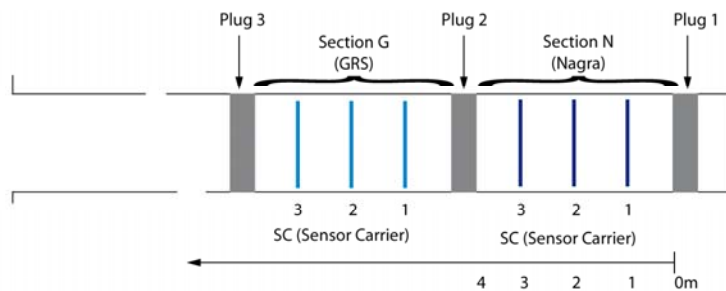


- Maximum heater temperature will be reached after 1 year
- Constant temperature at 140° for the next 2 years
- Strategy can be adapted

- Two independent isolated heaters of 4 m in steel liner
- Both power and temperature control

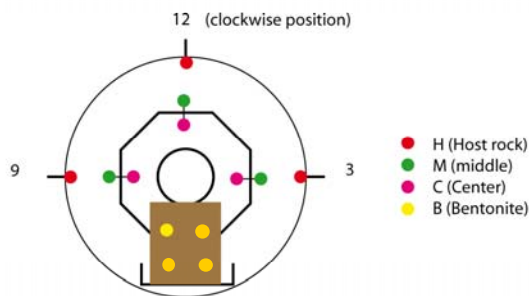


Instrumentation in the Engineered Barrier

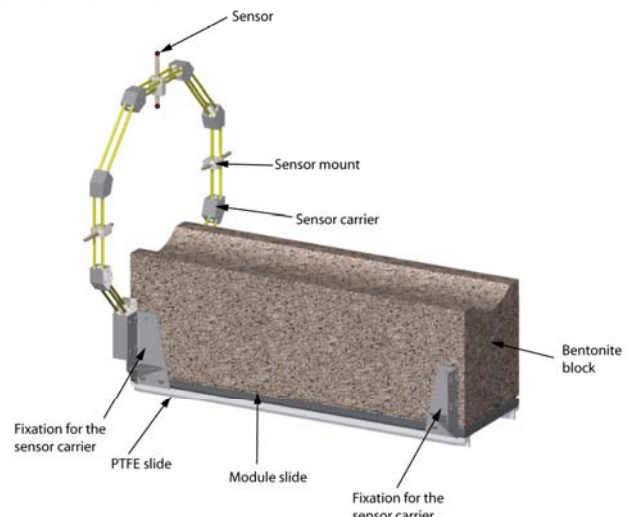


- Humidity and T° sensors
- Dense instrumentation lay-out:
 - 36 in granular material
 - 22 in blocks
 - 18 on interface
- Large T° gradient expected

Front view (inside the tunnel)

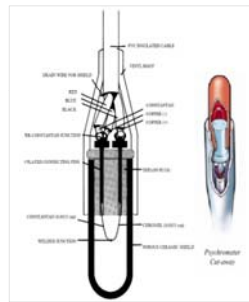
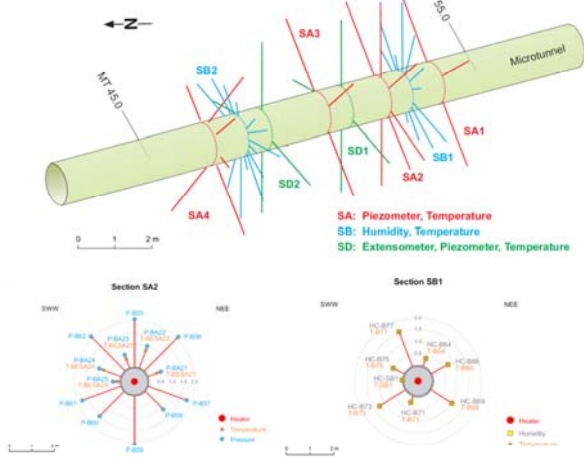


- Prefabricated modules facilitating emplacement

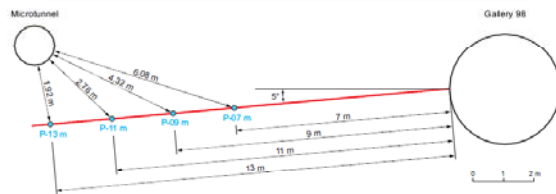


Instrumentation in the host rock

Close to microtunnel < 2 m

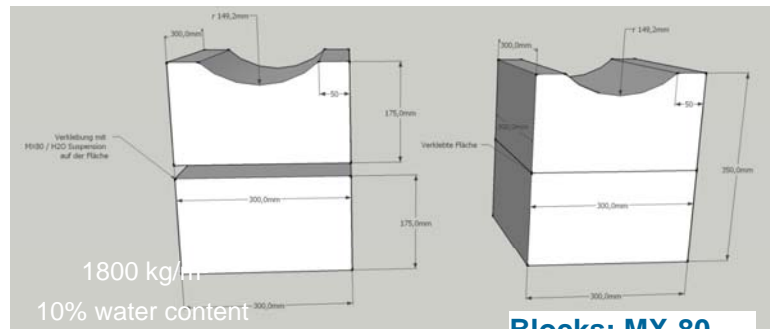
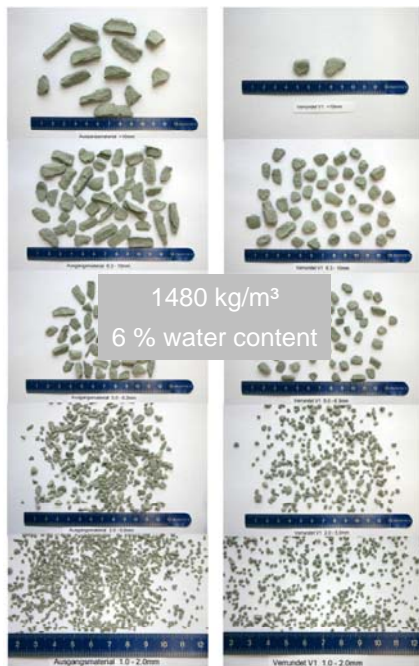


Further from microtunnel: boreholes from main gallery



Materials used

Section 1: MX80



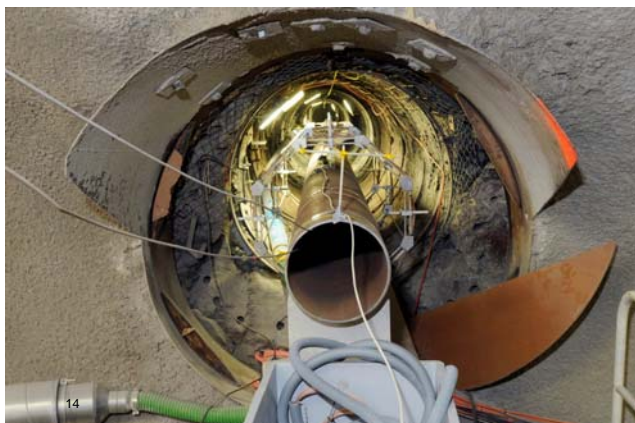
Section 2: Sand/bentonite (MX80) Max Grainsize : ca. 2 mm



Instrumentation in Opalinus Clay



Emplacement of instrumentation modules



Emplacement of granular bentonite by Auger



May 2011

Emplacement of the heaters – start in June 2011



Detail of the thermocouple positioning pieces.



Heater 2 on the platform



Insertion of the heater 1.

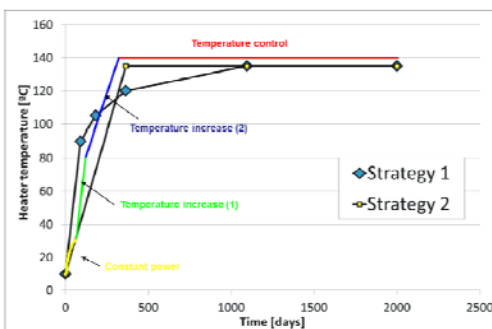


June 2011

Outline of this presentation

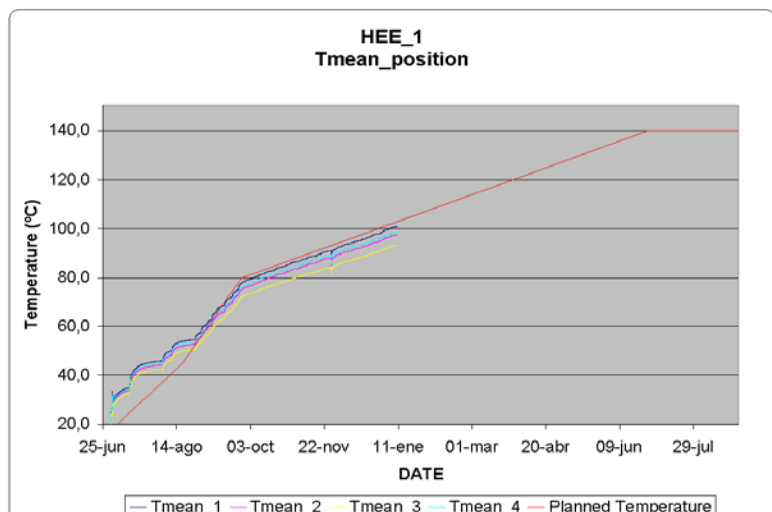
- Introduction to the experiment
- Construction and start of the experiment
- **Ongoing heating and monitoring since June 2011**
- Modelling strategy and results
- Conclusions so far

Implementation of the heating strategy

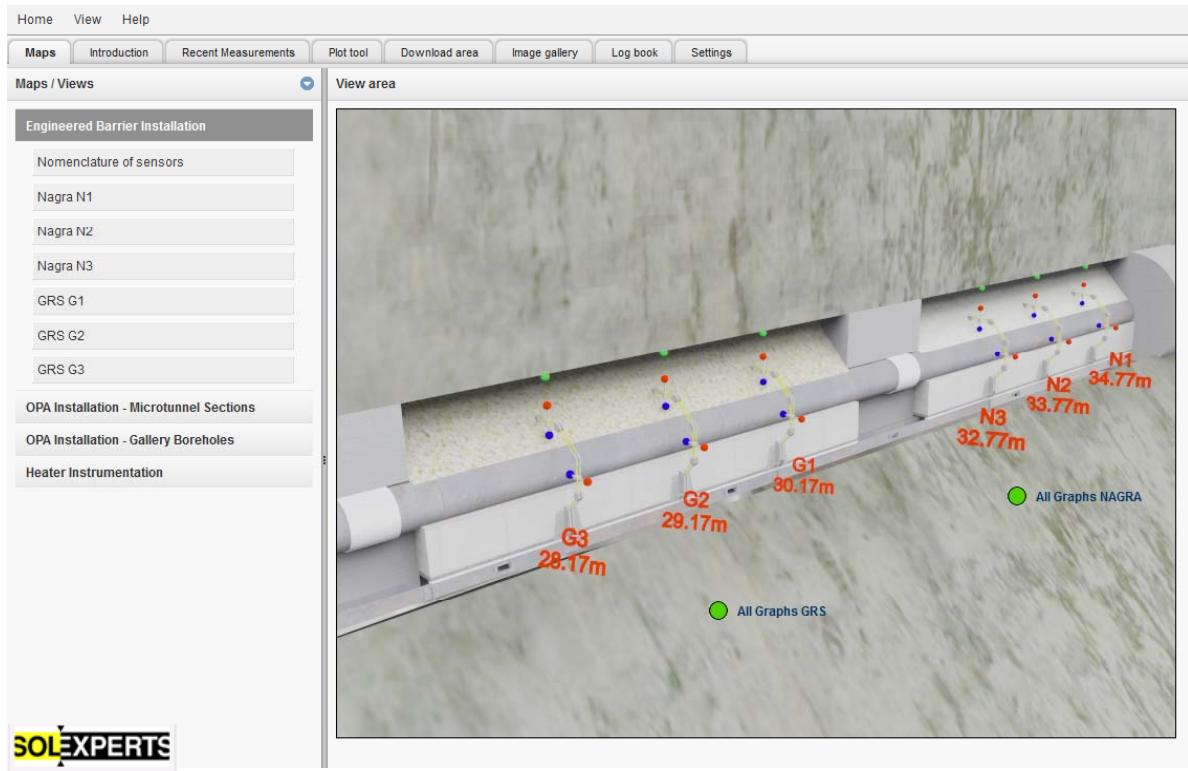


- **Current temperature evolution:
Now at ~120°C – 140°C in June 2012**

- **Heater strategy scaled down from expected canister heat output – temperature at canister surface**



First Monitoring results: WEBdavis – online access

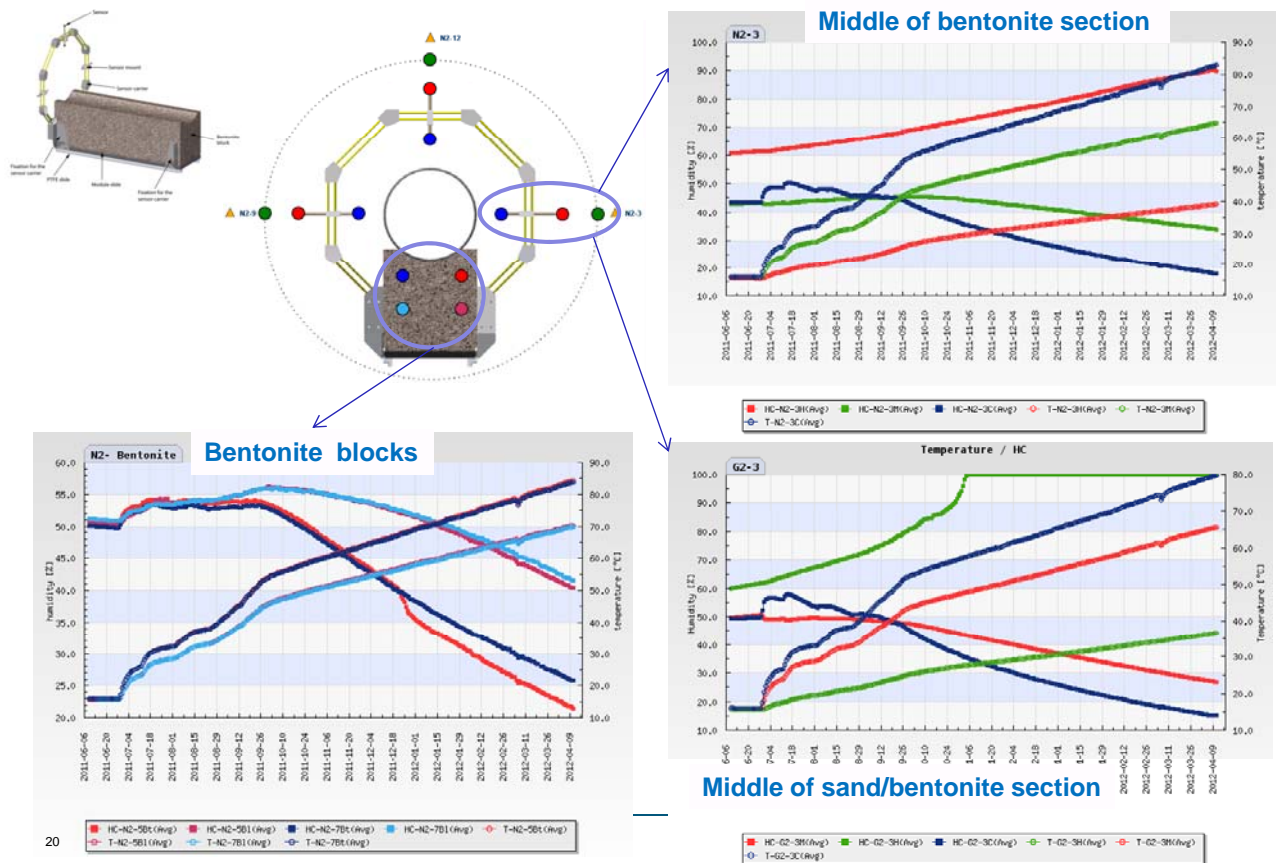


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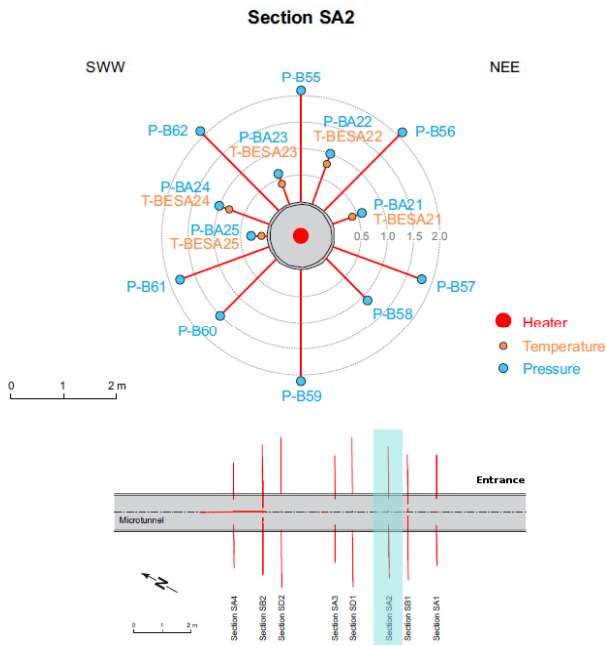
Current measurements in engineered barrier



20

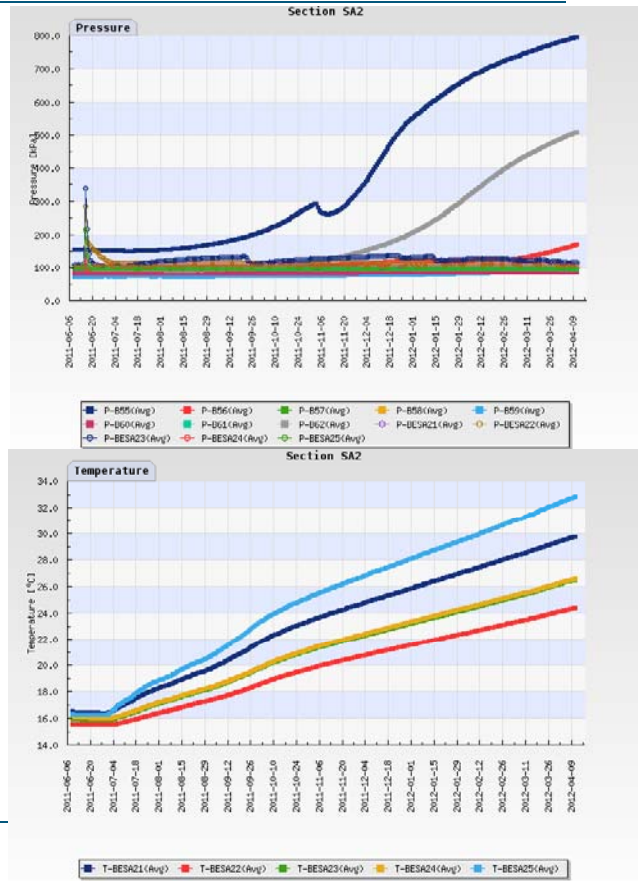
91

Current measurements in Opalinus Clay 1/2

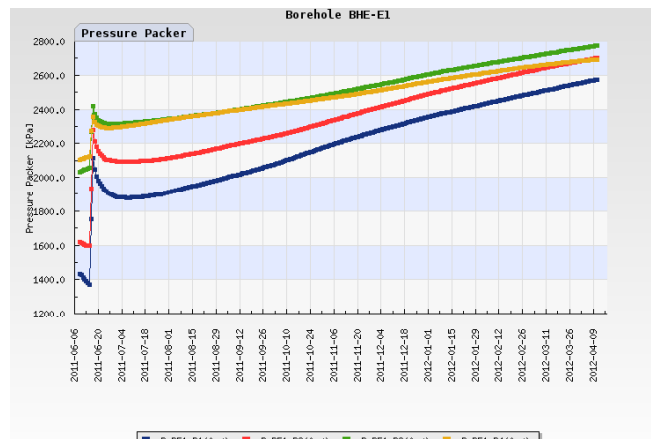
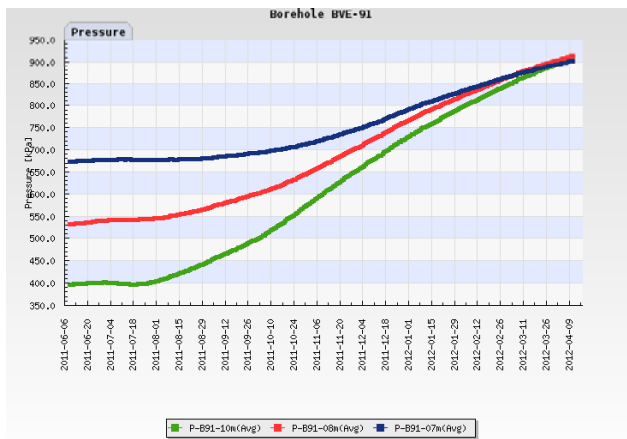
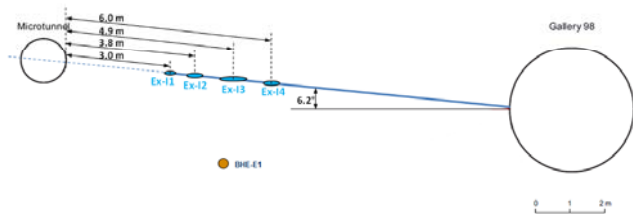
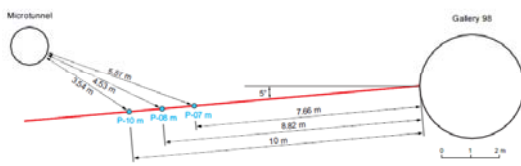


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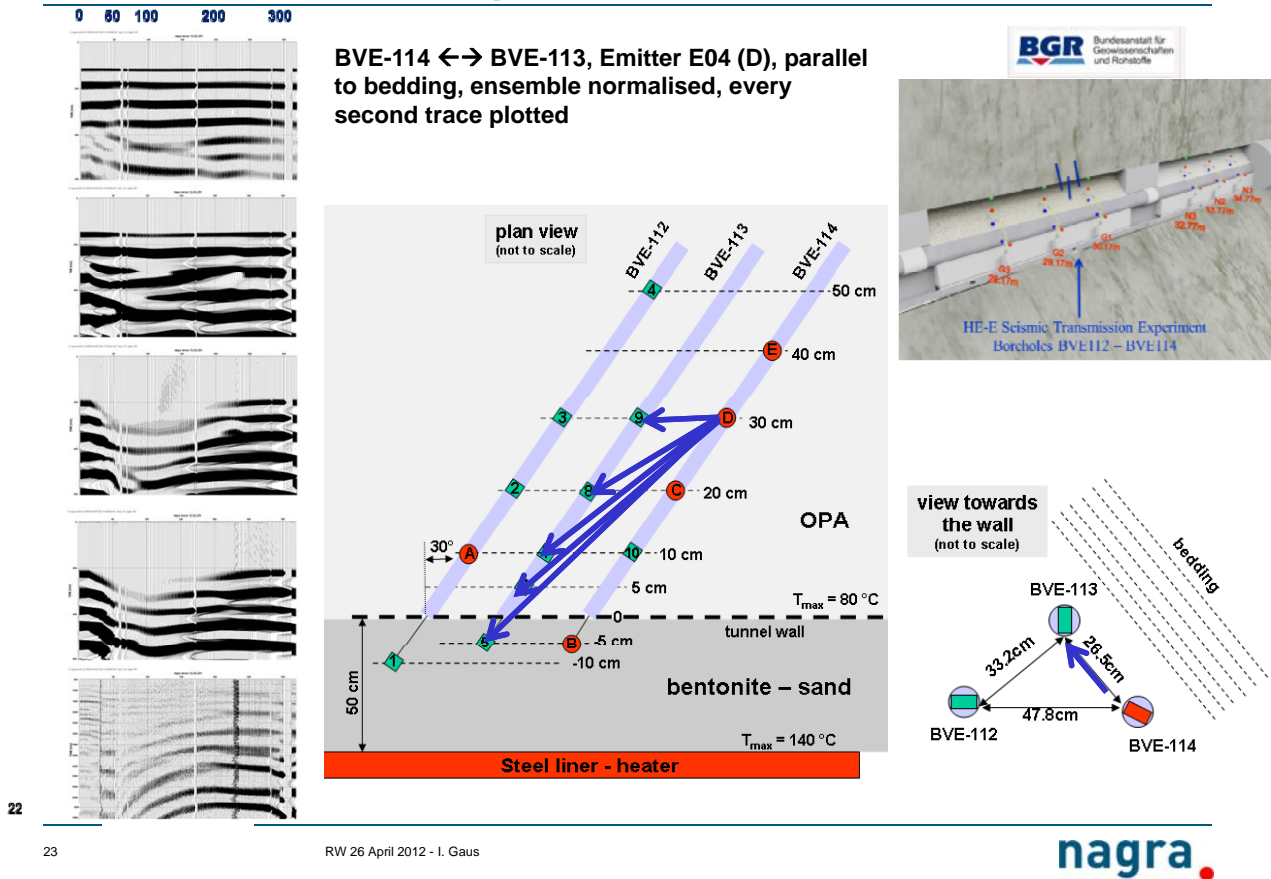
Current measurements in Opalinus Clay 2/2



22

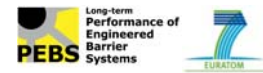
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Indirect monitoring: seismic transmission

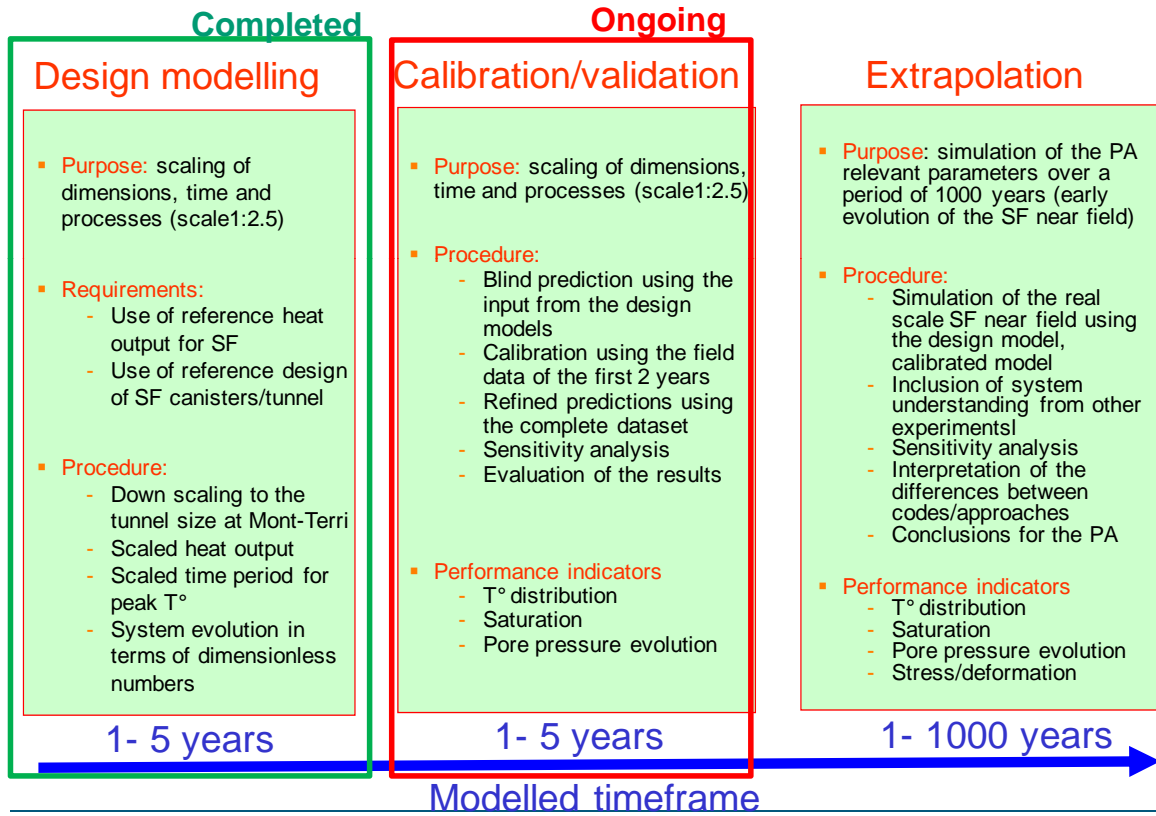


Outline of this presentation

- Introduction to the experiment
- Construction and start of the experiment
- Ongoing monitoring since June 2011
- **Modelling strategy and early results**
- Conclusions so far



Modelling strategy – 3 Teams – TH and THM



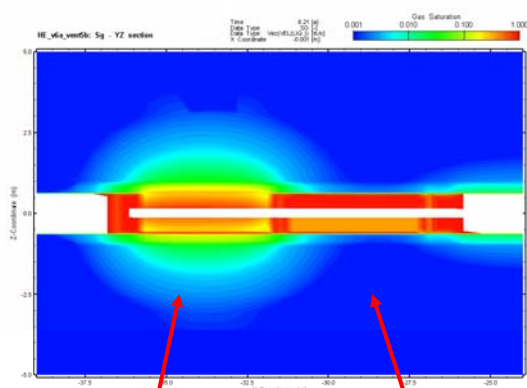
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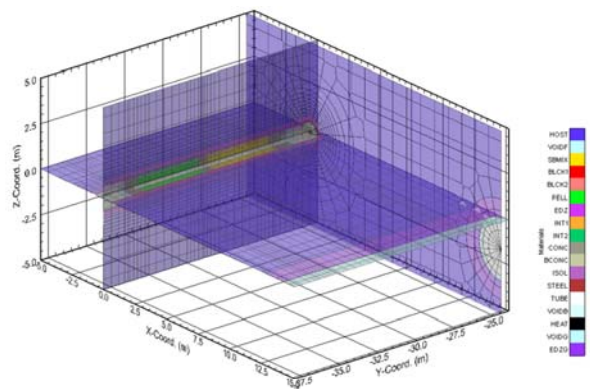
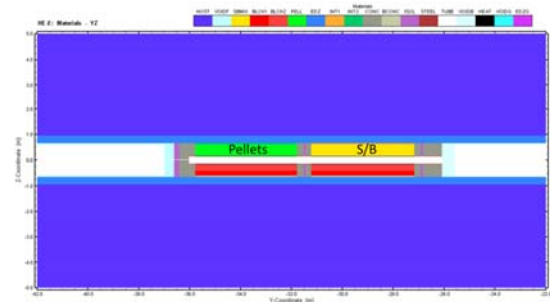
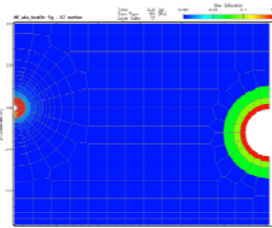
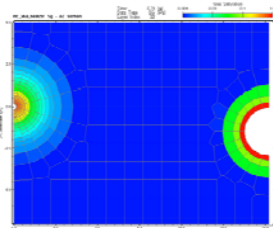
TOUGH (TH): first predictive calculations – as-built data

▪ Gas saturation after 6 years



Pellets

S/B

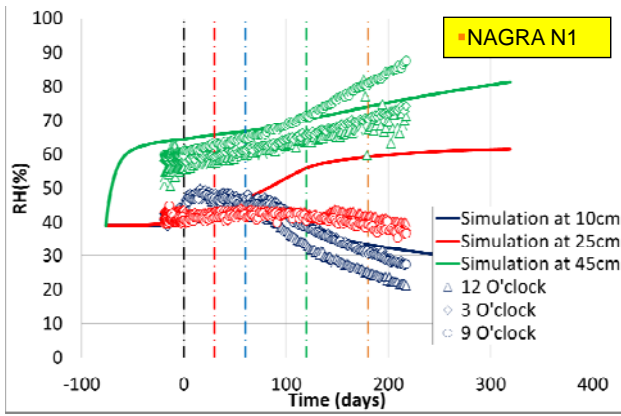


26

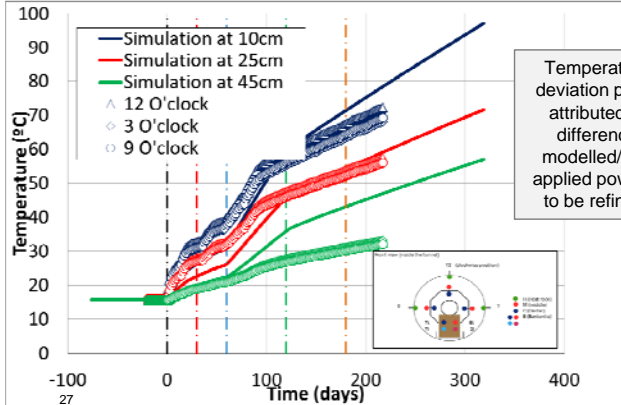
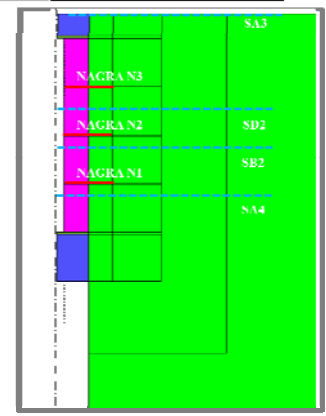
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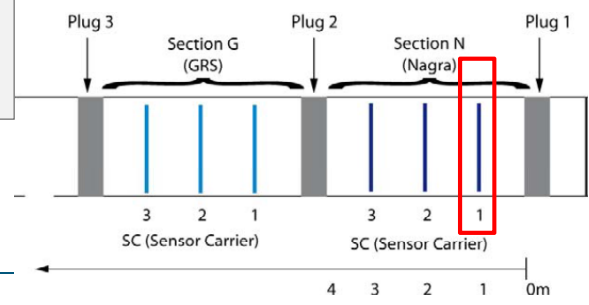
CodeBright (THM): first predictive calculations - as-built data



- Soil: Opalinus Clay
- bent: MX80
- insul: "gap"
- plug: concrete barrier



Temperature deviation partly attributed to difference modelled/real applied power – to be refined!



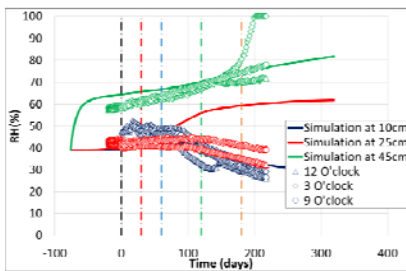
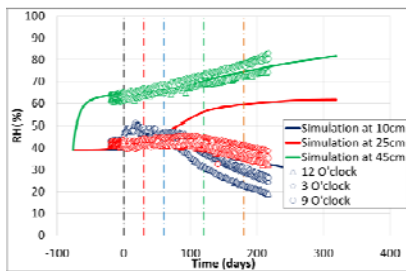
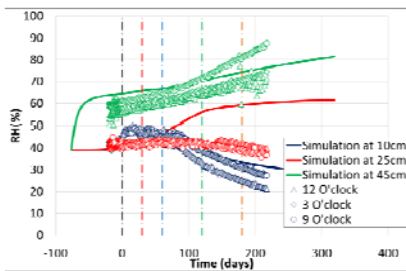
Code Bright: Simulation results against measurements

N1

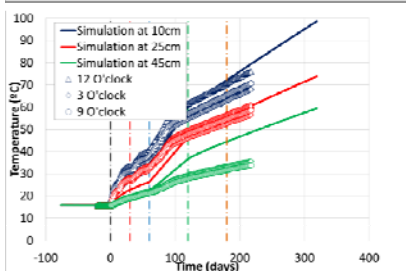
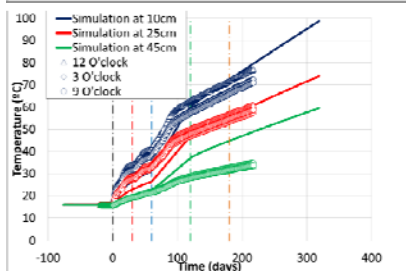
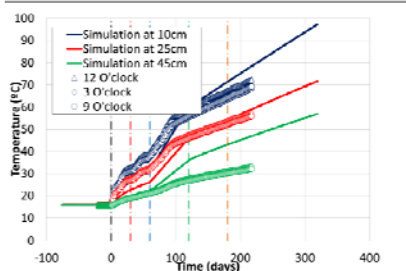
N2

N3

RH



Temperature



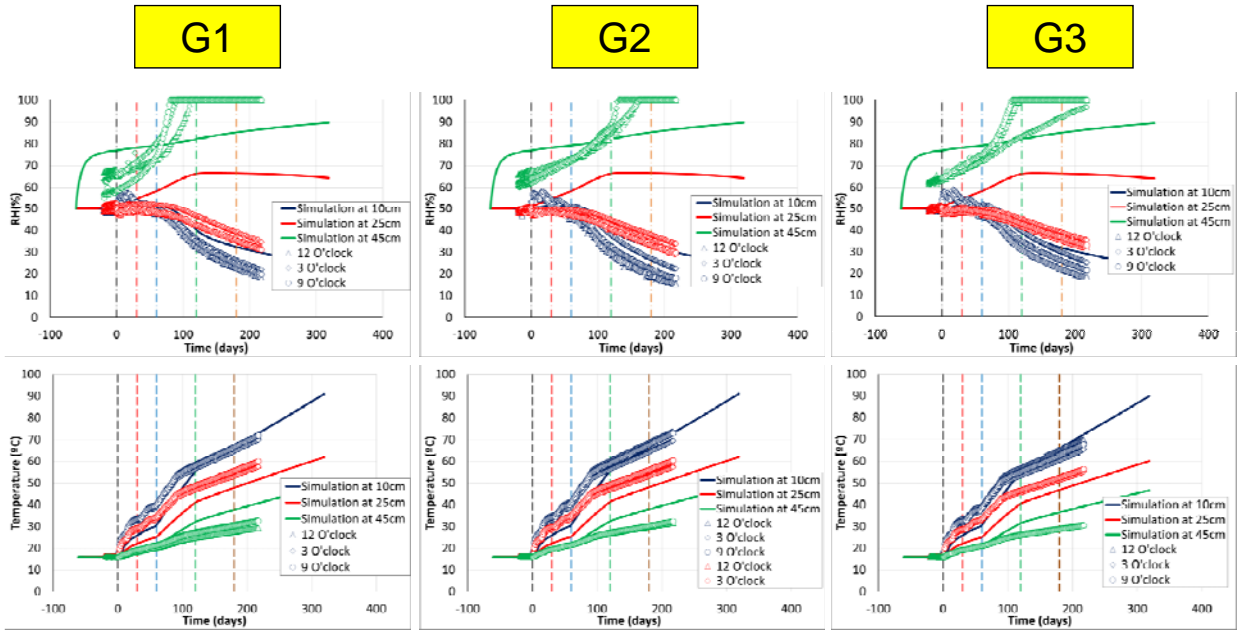
NAGRA – section: bentonite pellets



Code Bright: Simulation results against measurements

RH

Temperature



GRS – section: sand/bentonite

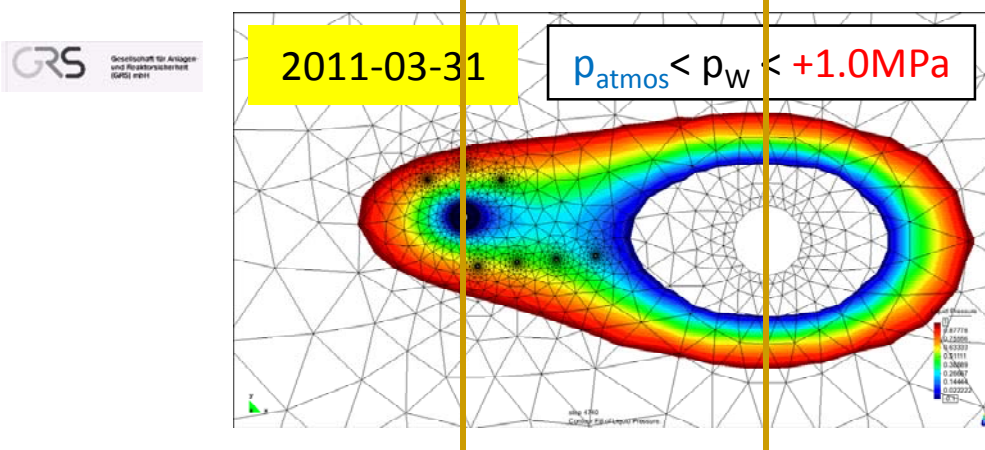
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Code Bright: plans for 3D THM modelling



- Design modelling illustrated the influence of Gallery 98 in terms of expected pressure evolution
- The impact is mostly restricted to one side of the microtunnel.
- This means the vertical plane through the microtunnel axis could be used as symmetry plane for a half-model, and two calculation runs (one with and one without Gallery 98) would give very similar information as one with a large model.



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- **Maximum heater temperature of 140°C will be reached in June 2012 – currently at 120°C – after that constant for at least 2 years**
- **Temperature increases as expected in EBS, slightly lower than predicted in the OPA**
- **OPA close to the microtunnel: no increases in pressure observed in most sensors – still slightly unsaturated close to the tunnel wall.**
- **Temperature in bentonite and sand/bentonite show similar evolution. All humidities in EBS decrease rapidly, apart from sand/bentonite – OPA interface.**
- **Onset of pressures increases due to thermal expansion at larger distance from the tunnel is observed (as predicted in the models) shortly after starting the heaters**

Acknowledgement

- *The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 249681*





PEBS Workshop for Regulatory Authorities

Overview of Modeling Tasks (WP3)

St-Ursanne, April 25 and 26, 2012



Fig. 1



St-Ursanne, April 25-26, 2012

WP3 Overview



Presentation Outline



- Background
- Structure and objectives of PEBS Work Package 3
- Overview of the modeling tasks 3.1 – 3.4
- Task 3.5 – long-term extrapolation
- Summary and outlook

Fig. 2



St-Ursanne, April 25-26, 2012

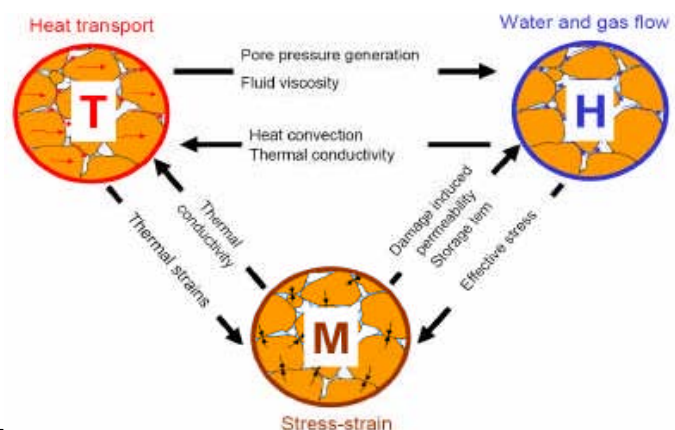
WP3 Overview

- In order to maintain isolation of the waste, the system has to meet requirements with regard to **hydraulic behaviour** and **mechanical, thermal, and chemical stability** over long periods of time (long-term safety assessment typically considers times of 10^5 years and more).
- Experimental evidence is only available for much shorter time periods. => The Thermal-Hydraulic-Mechanical-Chemical (**THMC**) **coupled processes in a repository have to be well understood**, so that a sound prediction of the future evolution of the repository can be undertaken.
- In-depth study of the behaviour and properties of the different materials present in the repository and their interaction are needed, in order to be able to **develop, qualify, and calibrate constitutive models** describing the evolution of the repository components and of the whole system.

Fig. 3

Process Types Potentially Occurring in a Repository

- **Mechanical:**
Stress/deformation behaviour of host rock and technical components, possibly time-dependent, e.g., creep deformation; fracturing and reconsolidation
- **Thermal:**
Heat flow and temperature increase as a consequence of decay heat production
- **Hydraulic:**
Pore water redistribution, de- / re-saturation of clay materials
- **Chemical:**
Corrosion of metallic or non-metallic components, chemical interaction at interfaces
- **TM coupled:**
Thermal expansion, viscosity changes
- **HM coupled:**
Dependence of mechanical state on pore pressure and saturation state, porosity change by compaction
- **HC coupled:**
Porosity/permeability change by chemical interaction (solution/precipitation)



THM-coupled phenomena (GENS et al., 2006)

Fig. 4

- WP1: **Analysis of system evolution** during early post closure period: Impact on long-term safety functions
- WP2: **Experimentation** on key EBS processes and parameters
- WP3: **Modeling** of short-term effects **and extrapolation** to long-term evolution
- WP4: Analysis of **impact on long-term safety** and guidance for repository design and construction
- WP5: Dissemination of results
- WP6: Project management

Fig. 5

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WP3 Overview

The overall objectives of WP3 are

- to perform coupled **HM, THM, and THMC analyses** to provide a sound basis **for the interpretation** of the various tests planned in the frame of the PEBS WP2
- to **develop new or improved models** as demanded by the calibration of computation results with the actual measured data, and
- to use the data and improved models for **extrapolation to long-term evolution** of the repository taking into account the scenarios defined in PEBS WP1 and to investigate model uncertainty and its impact on long-term prediction, thus providing input to PEBS WP4

Fig. 6

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WP3 Overview

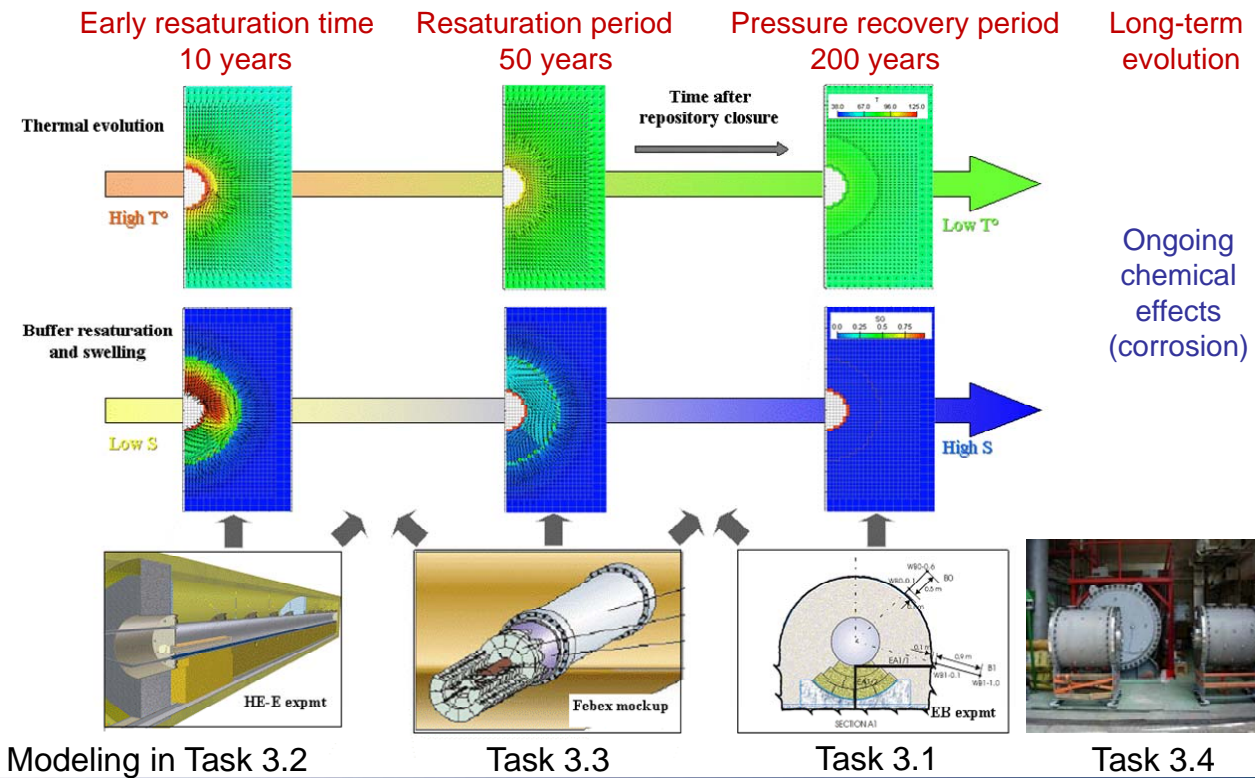


Fig. 7

Structure of WP3

- Task 3.1: **HM modeling** of the Mont Terri EB experiment (CIMNE, ENRESA)
- Task 3.2: **THM modeling** of the Mont Terri HE-E (CIMNE, ENRESA, TKConsult, NAGRA, GRS, BRIUG)
- Task 3.3: **THM modeling** of bentonite buffer (CIMNE, ENRESA, TKConsult, NAGRA, Clay Technology, SKB, BRIUG)
- Task 3.4: **THMC modeling** of various experiments (UDC, ENRESA, JAEA, BRIUG)
- Task 3.5: Long-term **extrapolation** (All teams)
 - To the end of the resaturation phase ($10^2 - 10^3$ years)
 - To the end of PA-considered time ($10^5 - 10^6$ years)
 - Natural analogues?

Fig. 8

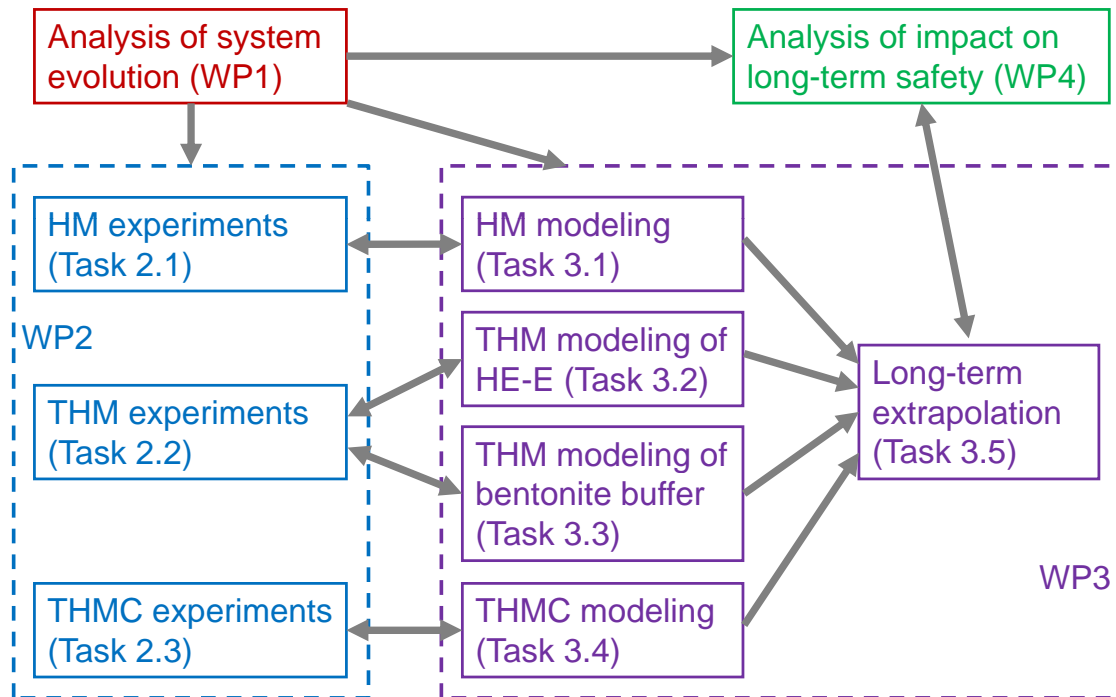


Fig. 9

Task 3.1: Objectives

- The HM modeling aims at providing a satisfactory scientific representation and a sound basis for **interpretation of the EB hydration phase** and of the dismantling data. New or improved constitutive laws (double structure approach, water density change) are developed and adjusted with the experimental data.

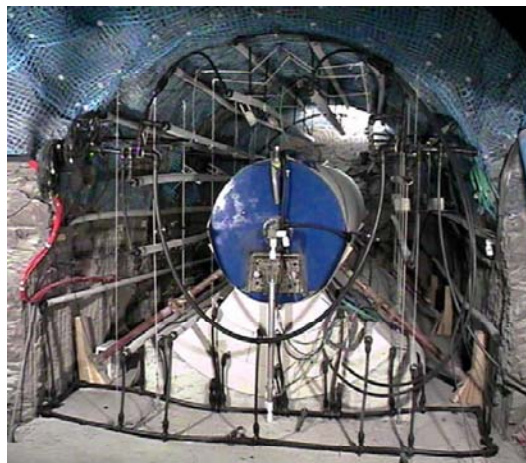
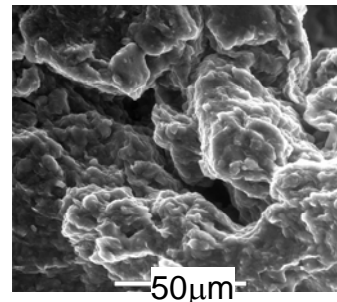
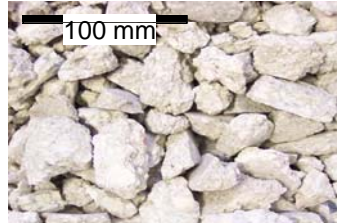


Fig. 10

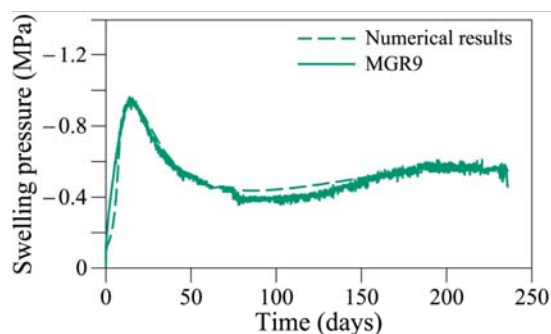
- Double structure approach: constitutive model for double porosity swelling clays
 - Two structural levels are considered: macrostructure and microstructure



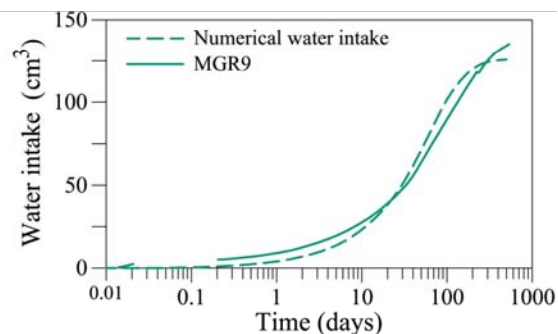
- Macrostructure model: use of conventional unsaturated soil model: BBM (Barcelona Basic Model)
- Microstructural model: empirical model relating volumetric strain and effective stress
- New step: non-equilibrium between microstructure and macrostructure

Fig. 11

- First simulations with the new approach showed good representations of experimental findings
- The model seems suitable for simulation of the EB



c)



f)

- Water density changes are currently being incorporated
- The final state of the barrier including dismantling effects is predicted and compared with the dismantling observations

Fig. 12

- **Scoping calculations** for the design of the **HE-E** to assure that the experiment lay-out meets the requirements regarding temperature evolution and that instrumentation is adequate
- **Interpretative modeling of the HE-E** by prediction/evaluation cycles with uncertainty assessment, concentrating on the thermal and thermomechanical behaviour in the early post-closure phase

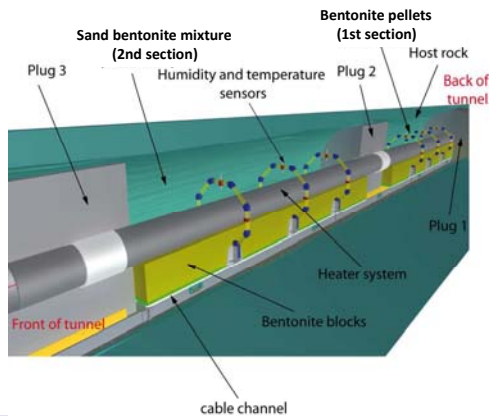
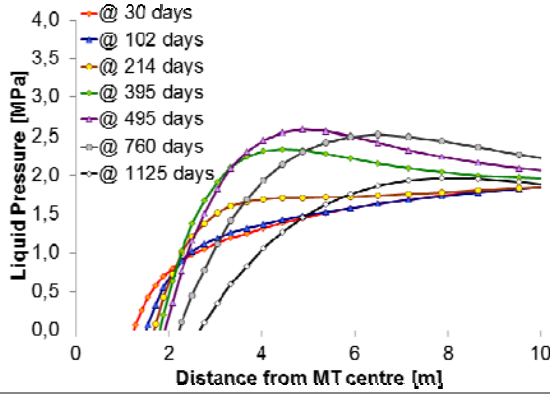


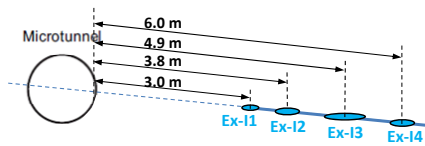
Fig. 13

- Scoping calculations of the HE-E have been finished
 - CIMNE: CODE_BRIGHT with a 2D-axisymmetric model, THM coupled calculation
 - GRS: CODE_BRIGHT with a 2D plane strain model, THM coupled calculation
 - TKConsult: TOUGH2 with a 3D model, TH calculation
 - Different modeling of the microtunnel history (draining)
 - Preliminary material properties
- Results:
 - Temperature increase at the microtunnel wall to 50-65 °C during the first year of heating, up to 72 °C after 3 years
 - Maximum pore pressures at >4 m distance from the microtunnel axis
 - Little water inflow into the buffer during experimental time: no swelling pressures expected

Fig. 14



Liquid pressure profiles after various heating times (CIMNE calculation)



Pressure evolution in the rock at different distances from the microtunnel (measurement)

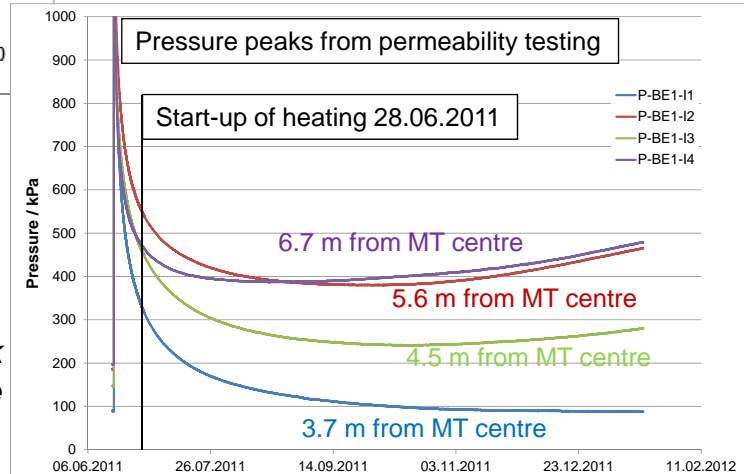


Fig. 15



- Development/validation of constitutive models and selection of parameters for the EB materials and the Opalinus clay
 - Respective laboratory tests on the buffer materials are currently going on
- Interpretative modeling of the HE-E test by the different modeling teams

Fig. 16



- Evaluation of existing **THM models for buffer** materials
- Incorporation of **new processes** into simulation of long-term lab experiments and development of **enhanced constitutive models**
- Simulation of long-term lab experiments and **extrapolation to large-scale in-situ tests**

Fig. 17

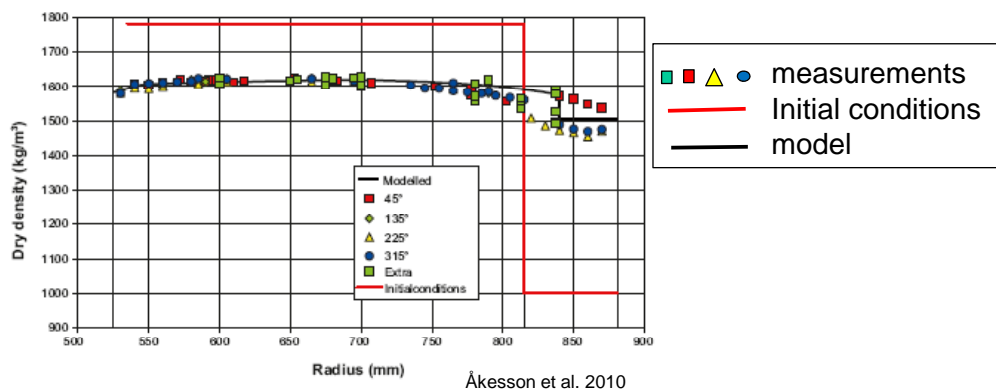


May 26th and 27th, 2011

Project Meeting, Work Package 3

Task 3.3: Evaluation of Existing Models

- Clay Technology analysed 11 models considering the bentonite buffer evolution. One of the models considering buffer homogenisation was a coupled THM model and the others were TH, HM or T models - the model was verified and can be used for other tasks in the project



Example result of modeling buffer homogenisation obtained with ABAQUS

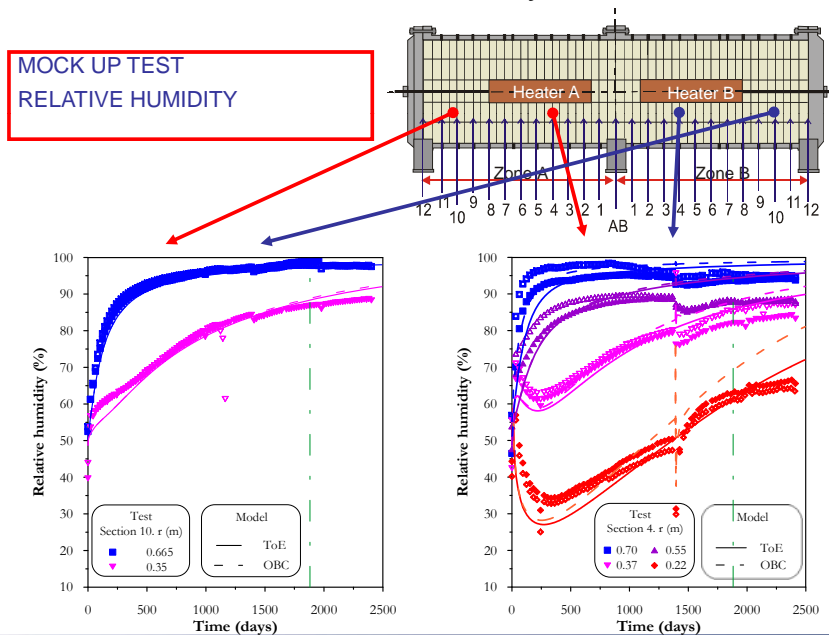
Fig. 18



May 26th and 27th, 2011

Project Meeting, Work Package 3

- CIMNE performed long-term THM modeling of the FEBEX mock-up test and evaluated several non-conventional models for better simulation of the bentonite hydration



Measured and calculated relative humidity in the FEBEX mock-up taking into account thermo-osmosis

Fig. 19

May 26th and 27th, 2011

Project Meeting, Work Package 3

- SKB/Clay Technology will use their models for long-term simulation and evaluation of uncertainties
- NAGRA/TKConsult will select relevant experiments (e.g., FEBEX in situ), for extrapolation until full saturation (or equilibrium)
- CIMNE will perform long-term THM modeling of CIEMAT cell tests

Fig. 20

May 26th and 27th, 2011

Project Meeting, Work Package 3

- Development of models accounting for **different types of water** and incorporating **porosity change** resulting from swelling in THC code; testing by simulation of PEBS experiments and lab tests performed in the frame of NF-PRO
- Validation of an existing THMC code by simulation of PEBS experiments

Fig. 21



May 26th and 27th, 2011

Project Meeting, Work Package 3

- UDC has developed advanced multiple continua models for clay barriers by improving current THC(m) models. The following improvements were made:
 - A dual micro-macro formulation has been developed to account for different types of water and pores
 - A state-surface approach has been used to model the swelling
 - Reactive gases such as O₂, CO₂ and H₂ are accounted for
- The improved model was benchmarked against other codes and applied for different experiments
- Next steps:
 - Simulate 60 cm-column experiments of CIEMAT
 - Simulate tests on bentonite-concrete and canister-bentonite interface

Fig. 22



May 26th and 27th, 2011

Project Meeting, Work Package 3

- Assessment of the results of Task 3.1 - 3.4 regarding their implications for different time and space scales
- **Identification of the significant processes** in the resaturation phase & afterwards
- Development or modification of the available **formulations to incorporate phenomena and processes deemed to be relevant** for long-term predictions
- **Performance of coupled numerical analysis** for long-term evolution of the engineered barrier system in the repository
- **Evaluation of the model uncertainty** and its implications for long-term prediction
- Compilation and evaluation of the usefulness of natural analogues for providing support, testing and validation of long-term predictions of current THMC models

Fig. 23

WP1: Compilation of important processes, possibly exhibiting uncertainty in their formulation, as seen from the various national programmes



Task 3.5: Evaluation: Which of these processes are addressed in PEBS WP2 and WP3?



WP4: Selection of modeling cases for extrapolation, proposal on case variants



Task 3.5: Definition of case variants, performance of long-term simulations, uncertainty evaluation, processing of results for WP4



WP4: Evaluation

Fig. 24

Important processes considered in PEBS (marked in red: Processes contain uncertainties in their description)

| Process | Re-saturation and thermal period | Long-term after re-s. and thermal period | Considered in Task |
|---------------------------------------|----------------------------------|--|--------------------|
| Heat transport | XXX | XXX | 3.2, 3.3 |
| Water uptake | XXX | | 3.1, 3.3, 3.4 |
| Water transport (sat.cond.) | XXX | XXX | 3.3, 3.4 |
| Piping/erosion | XXX | | 3.3 |
| Swelling/homogenization | XXX | XXX | 3.1, 3.3, 3.4 |
| (Thermal) osmosis | XXX | XXX | 3.3 |
| Transport of solutes | XXX | XXX | 3.4 |
| Thermal alteration | XXX | XXX | 3.4 |
| Geochemical evolution | XXX | XXX | 3.4 |
| Cementation / montmorillonite transf. | XXX | XXX | 3.4 |
| Corrosion product interaction | XXX | XXX | 3.4 |
| Concrete interaction | XXX | XXX | 3.4 |

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WP3 Overview

- The processes which exhibit uncertainties are the most candidate for the extrapolation consideration
- Substantial data to improve their description should be provided within PEBS
- The modeling cases to be considered should interest more than just one PEBS partner

- **Water uptake in the buffer ($T < 100\text{ °C}$)**
 - Input data from Task 2.1 & 2.2, modeling in Task 3.1 & 3.3
- **Thermal evolution of the buffer ($T > 100\text{ °C}$)**
 - Input data from Task 2.2, modeling in Task 3.2
- **Hydro-mechanical evolution of the buffer**
 - Input data from Task 2.1 & 2.2, modeling in Task 3.1, 3.2 & 3.3
- **Geochemical evolution**, especially at interfaces (canister – bentonite and bentonite – concrete)
 - Input data from Task 2.3, modeling in Task 3.4

Fig. 27



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WP3 Overview

Current Status of Task 3.5

- The models for the relevant processes are in principle existing and will be used for long-term simulation. Such models include, e.g.
 - Non-Darcy flow (threshold and critical gradient)
 - Thermo-osmosis
 - Double structure model to account for microfabric evolution
 - Different types of water in macro- and micropores
- They will be checked against the data from the experiments, which are already providing, confirming or improving a wide variety of parameters.
- Currently, the case variants for the extrapolation simulations are being defined.

Fig. 28



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WP3 Overview

- Check of the available processes or process formulations for completeness (“new” processes?) and necessity
 - By using different formulations for the same experiments
 - By modeling of the PEBS WP2 (or other) experiments (for HE-E in prediction-interpretation cycles)
- Check of the necessity and suitability of formulations and parameters
 - By using the same formulations/parameters for different experiments (as far as reasonable)
- Check of sensitivity of parameters
 - By parameter variation, long-term simulation and comparison of results

Fig. 29



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WP3 Overview

- Numerical modeling is an integral part of the PEBS project. Although all process modeling is concentrated in one work package, there is a very close interaction with the other work packages.
- Besides the prediction/interpretation modeling of the various experiments performed in the frame of PEBS, a special task is the extrapolation to time scales not accessible by experimentation. This has direct impact on long-term safety considerations.
- By the end of PEBS,
 - Improved process models will be available and confirmed
 - Improved and confirmed parameters of buffer materials will be available and the models will be calibrated
 - Uncertainties in repository long-term behaviour will have been reduced

Fig. 30



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WP3 Overview

The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 249681

Fig. 31

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WP3 Overview

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Fig. 32

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WP3 Overview



Coupled thermal-hydraulic-chemical modelling taking into account some mechanical effects

PEBS Workshop for Regulatory Authorities

St. Ursanne, April 25th and 26th, 2012



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Regulatory Authority Workshop



Outline



- Introduction
- Objectives
- Coupled THC(m) models
 - ✓ Model description
 - ✓ Model testing
- Long-term evolution and simulation
 - ✓ Integrated analysis of THCM data
 - ✓ Natural analogs
 - ✓ Long-term simulations
- Conclusions

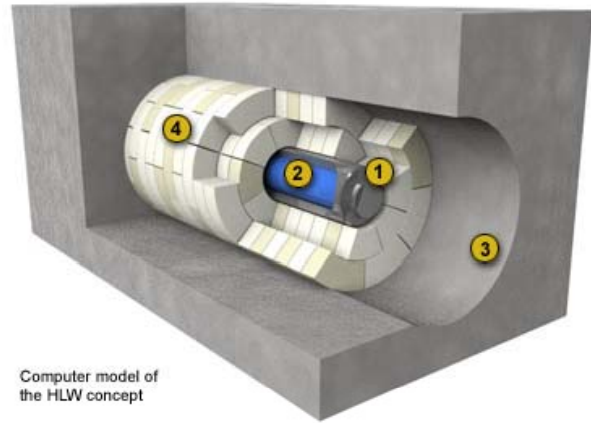
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- Engineered barrier system
 - Canister
 - Buffer & Barrier
 - Liner
- European R&D projects on



Computer model of the HLW concept

- FEBEX I, II
- BENIPA
- NFPRO
- **PEBS: Long-term performance of the Engineered Barrier Systems (EBS) (2010-2014)**
 - *The main aim is to evaluate the sealing and barrier performance of the EBS with time, through development of a comprehensive approach involving experiments, model development and consideration of the potential impacts on long-term safety functions*

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Hydrodynamic and thermal transient stages in the EBS

- **EBS water saturation:** from 20 to 100 years
- **EBS pressure equilibration:** 200 years
- **EBS thermal transient**
 - Thermal gradients within the EBS are expected to dissipate after 10^3 years
 - The thermal pulse will last for 10^4 years

Geochemical transient stages in the EBS

- Geochemical transient associated with the thermal and saturation stages:
 - Chemical processes triggered by water saturation
 - Chemical reactions caused by the thermal pulse
- Solute diffusion across the EBS-geosphere interface
- Geochemical evolution of major aqueous chemical species within the EBS
- Interactions of corrosion products & bentonite
- Interactions of concrete & bentonite
- Radionuclide migration, sorption and retardation

Objectives

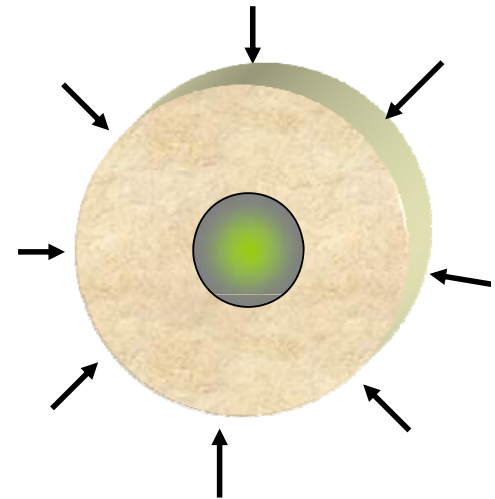
- Improve current THC models to
 - Account for different types of waters and pores
 - Account for the porosity changes caused by swelling phenomena → THCM model
 - Account for reactive gases $O_{2(g)}$, $CO_{2(g)}$, $H_{2(g)}$
- Test THCM model with lab and in situ tests
 - NFPRO and FEBEX tests
 - FEBEX mock-up and in situ tests
 - Heating and hydration tests
 - Interface tests: Canister/bentonite & concrete-bentonite
 - PEBS tests
 - Corrosion tests
 - Concrete-bentonite tests
 - New corrosion-concrete tests

- Study the long-term prediction ability of current THMC models
 - Integrated analysis of water uptake, temperatures, & chemical concentration data from different space and time scales
 - Natural analogs
 - Update the numerical simulation of the long-term geochemical evolution of the EBS



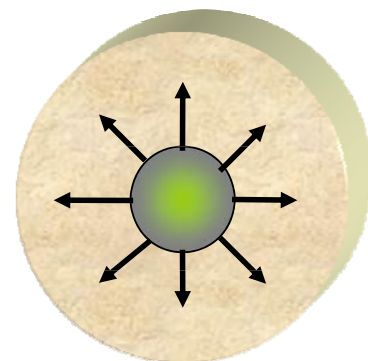
Flow processes

- Saturated-unsaturated medium
- Two-phase flow
 - Liquid (water, solutes, gases)
 - Gas
 - Air
 - Vapor
 - Other gases: $O_{2(g)}$, $CO_{2(g)}$, $H_{2(g)}$
- Evaporation and condensation
- Non-isothermal
 - Temperature dependence of hydrodynamic parameters
- Coupled Onsager processes
 - Chemical osmosis
 - Thermal osmosis



Thermal processes

- Conduction
- Convection
- Evaporation (heater/bentonite) and condensation



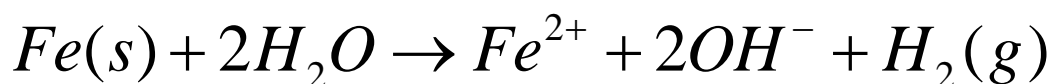
Solute transport processes

- Advection
- Dispersion
- Molecular diffusion

Geochemical system

| | |
|----------------------|--|
| Primary species | H ₂ O, H ⁺ , Ca ²⁺ , Mg ²⁺ , Na ⁺ , K ⁺ , Cl ⁻ , SO ₄ ²⁻ , HCO ₃ ⁻ , SiO ₂ (aq), O ₂ (aq), Fe ²⁺ |
| Aqueous complexes | OH ⁻ , CaSO ₄ (aq), CaCl ⁺ , MgCl ⁺ , NaCl(aq), MgHCO ₃ ⁺ , NaHCO ₃ (aq), CaHCO ₃ ⁺ , MgCO ₃ (aq), CaCO ₃ (aq), CO ₂ (aq), CO ₃ ²⁻ , KSO ₄ ⁻ , MgSO ₄ (aq), NaSO ₄ ⁻ , HSiO ₃ ⁻ , NaCO ₃ ⁻ , NaHSiO ₃ (aq), KCl(aq), CaCl ₂ (aq), CaH ₃ SiO ₄ ⁺ , CaOH ⁺ , MgH ₂ SiO ₄ (aq), MgH ₃ SiO ₄ ⁺ , HS ⁻ , HSO ₄ ⁻ , Fe(OH) ₂ ⁺ , Fe(OH) ₃ (aq), Fe(OH) ₄ ⁻ , Fe ³⁺ , H ₆ (H ₂ SiO ₄) ₄ ²⁻ , CaH ₂ SiO ₄ (aq), FeCO ₃ (aq), FeHCO ₃ ⁺ , Mg(H ₃ SiO ₄)(aq), NaOH(aq), H ₂ (aq) |
| Minerals & gases | calcite, quartz, gypsum/anhydrite magnetite, siderite, goethite, Fe(s) O ₂ , CO ₂ |
| Exchangeable cations | Ca ²⁺ Mg ²⁺ Na ⁺ K ⁺ Fe ²⁺ |

Steel canister corrosion



Geochemical system

| Cation exchange | $K_{\text{Na-cation}}$ |
|--|------------------------------|
| $\text{Na}^+ + \text{X-K} \Leftrightarrow \text{K}^+ + \text{X-Na}$ | 0.138 |
| $\text{Na}^+ + 0.5\text{Ca-X}_2 \Leftrightarrow 0.5\text{Ca}^{2+} + \text{Na-X}$ | 0.292 |
| $\text{Na}^+ + 0.5\text{Mg-X}_2 \Leftrightarrow 0.5\text{Mg}^{2+} + \text{Na-X}$ | 0.280 |
| $\text{Na}^+ + 0.5\text{Fe-X}_2 \Leftrightarrow 0.5\text{Fe}^{2+} + \text{Na-X}$ | 0.5 |
| $\text{Na}^+ + \text{X-H} \Leftrightarrow \text{H}^+ + \text{X-Na}$ | $3.16 \cdot 10^{-5}$ |
| Surface complexation | $\text{Log } K_{\text{int}}$ |
| $\text{SOH}_2^+ \Leftrightarrow \text{SOH} + \text{H}^+$ | -5.8 |
| $\text{SO}^- + \text{H}^+ \Leftrightarrow \text{SOH}$ | 7.9 |
| $\text{SOFe}^+ + \text{H}^+ \Leftrightarrow \text{SOH} + \text{Fe}^{2+}$ | 5.0 |

Porewater chemical composition

| Primary species | Bentonite | Granite |
|---------------------------|-----------------------|-----------------------|
| Ca^{2+} | $3.101 \cdot 10^{-2}$ | $1.522 \cdot 10^{-4}$ |
| Cl^- | $2.756 \cdot 10^{-1}$ | $3.949 \cdot 10^{-4}$ |
| Fe^{2+} | $6.583 \cdot 10^{-5}$ | $1.791 \cdot 10^{-8}$ |
| pH | 6.435 | 7.825 |
| HCO_3^- | $1.689 \cdot 10^{-3}$ | $5.049 \cdot 10^{-3}$ |
| K^+ | $1.507 \cdot 10^{-3}$ | $5.371 \cdot 10^{-5}$ |
| Mg^{2+} | $3.473 \cdot 10^{-2}$ | $1.604 \cdot 10^{-4}$ |
| Na^+ | $1.841 \cdot 10^{-1}$ | $4.350 \cdot 10^{-3}$ |
| Eh (V) | -0.059 | -0.188 |
| $\text{SiO}_2(\text{aq})$ | $3.761 \cdot 10^{-4}$ | $3.761 \cdot 10^{-4}$ |

– Bentonite porewater is more mineralized than granite water

Mechanical processes

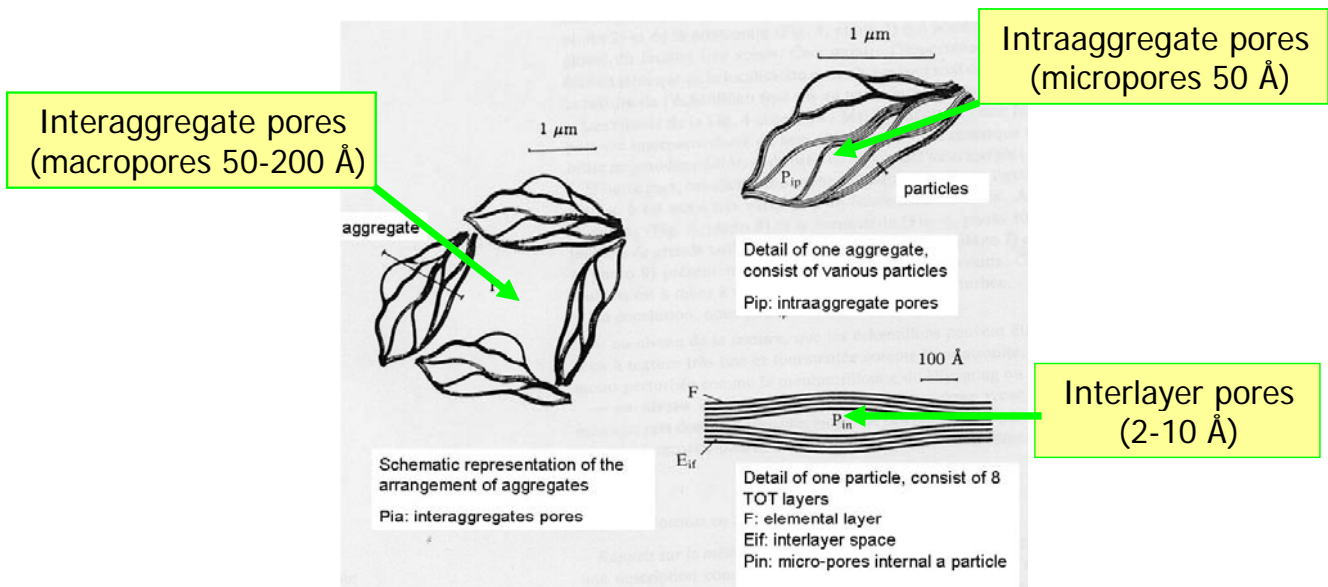
- Equilibrium equation

$$\nabla \cdot (\Delta \sigma' + \Delta p^g \delta) + \Delta \rho g \mathbf{k} = 0$$

- Bentonite swelling
 - State surface approach of Lloret & Alonso (1985)

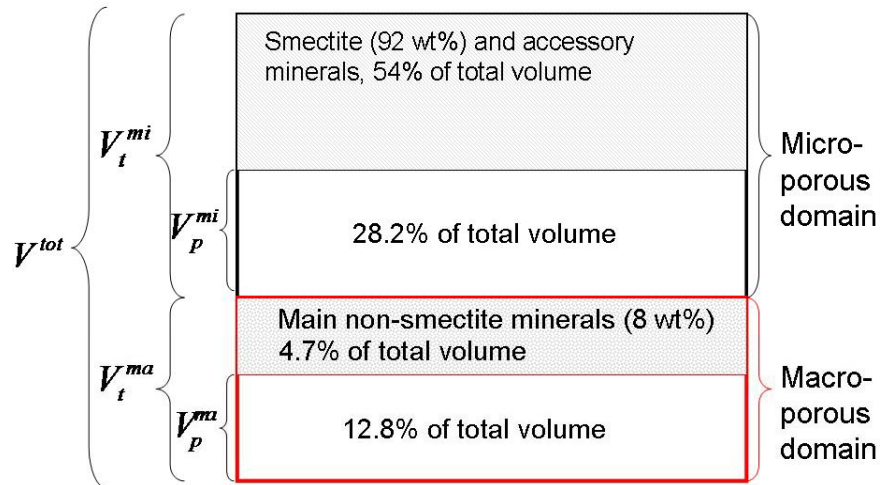
$$e = A + B \ln \sigma' + C \ln(\psi + p^a) + D \ln \sigma' \ln(\psi + p^a)$$

Multiple porosity structure of bentonite



schematic representation of types of pores (Touret et al., 1990)

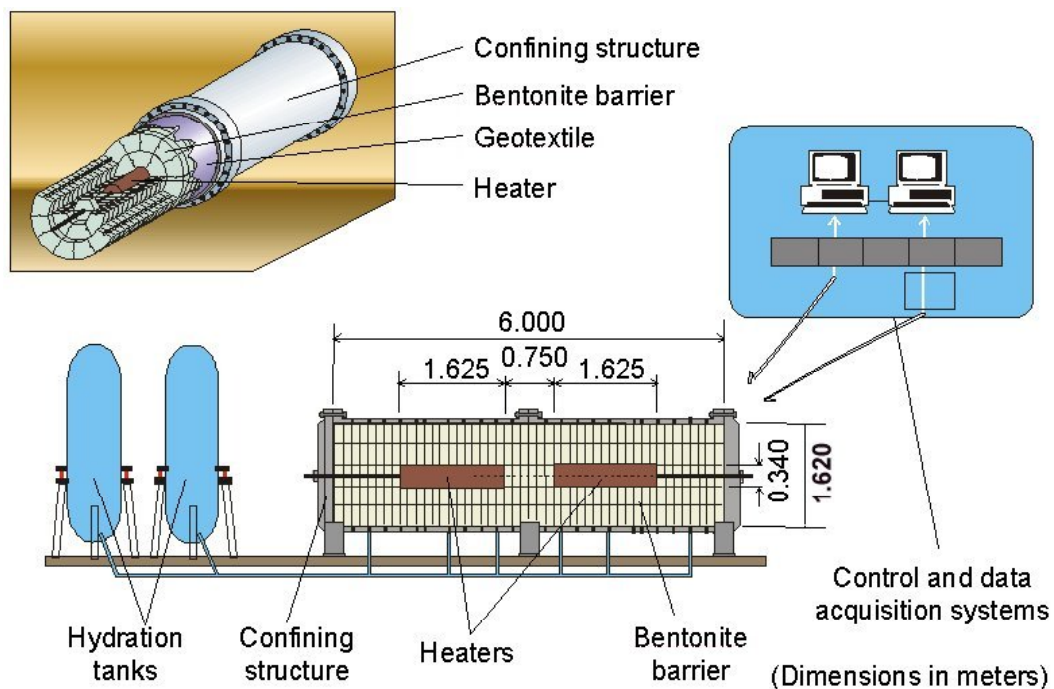
Dual porosity conceptual model: macro- and micro-porous domains



f^{ma} is 17.5%

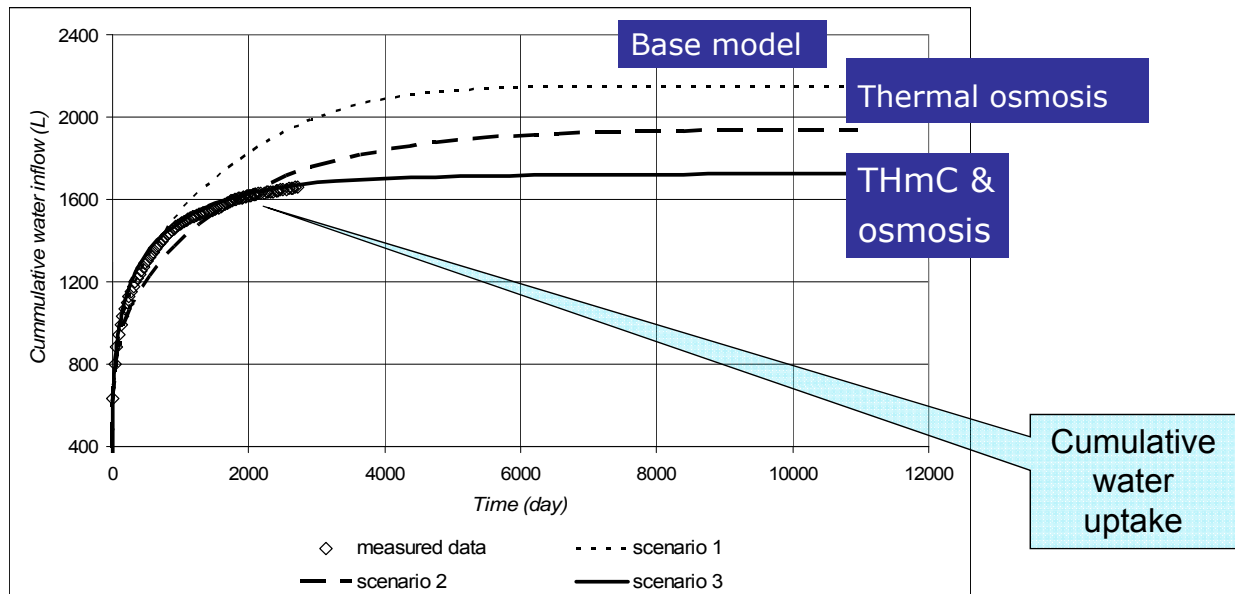
THMC model testing: mock-up test

Extend the THC(m) model of the FEBEX mock up test from 7 to 14 years (Zheng & Samper JPCE 2008)



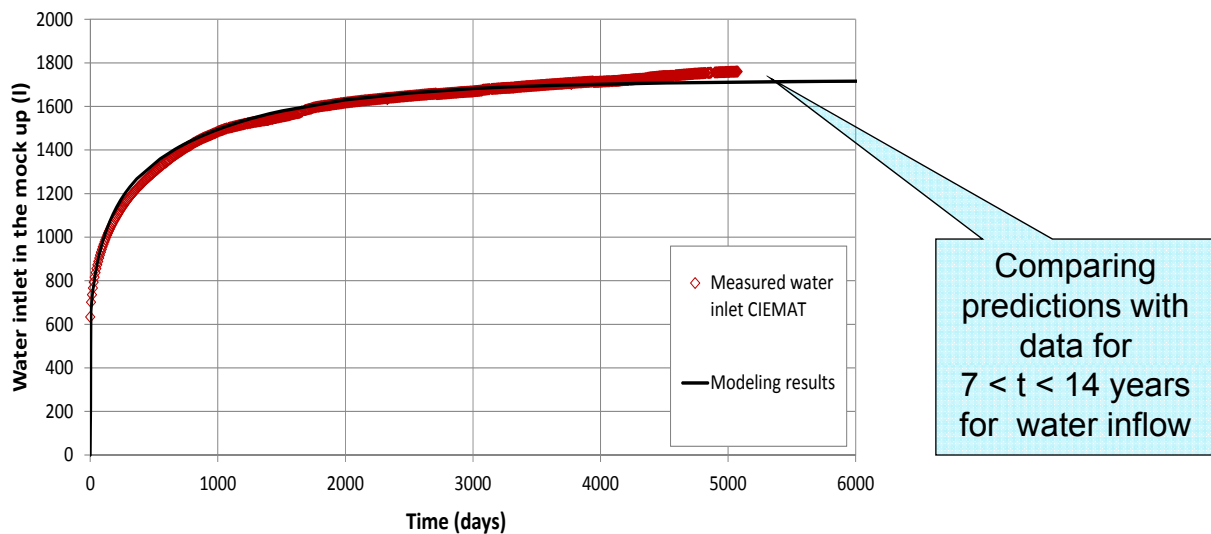
THMC model testing: mock-up test

Extend the THC(m) model of the FEBEX mock up test from 7 to 14 years (Zheng & Samper JPCE 2008)



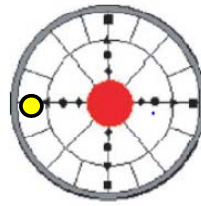
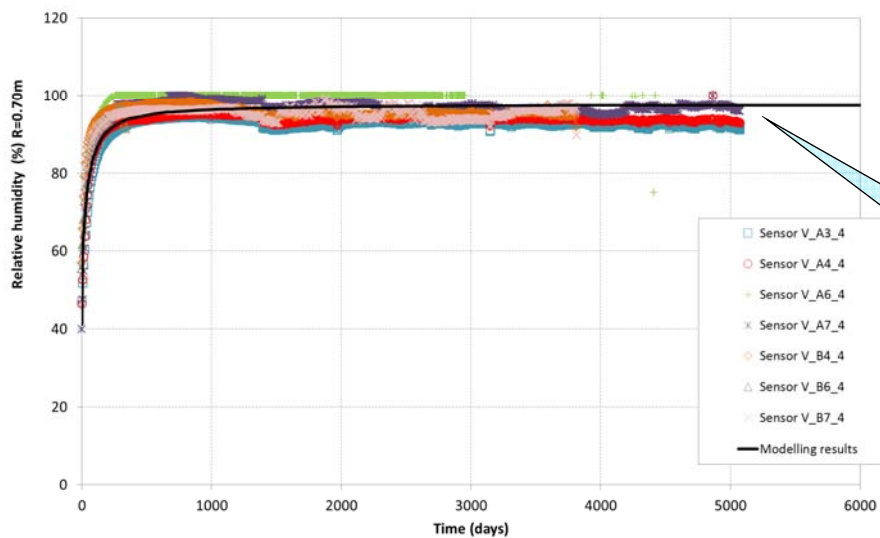
THMC model testing: mock-up test

Extend the THC(m) model of the FEBEX mock up test from 7 to 14 years



THMC model testing: mock-up test

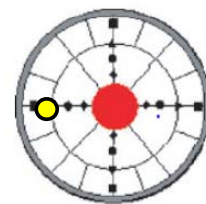
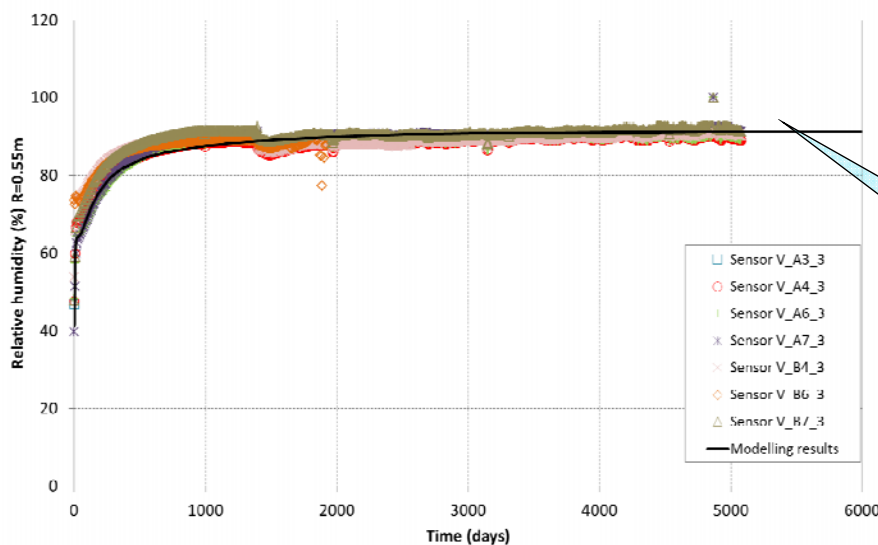
Extend the THC(m) model of the FEBEX mock up test from 7 to 14 years



Comparing predictions with data for $7 < t < 14$ years
RH @ $r = 0.70$ m

THMC model testing: mock-up test

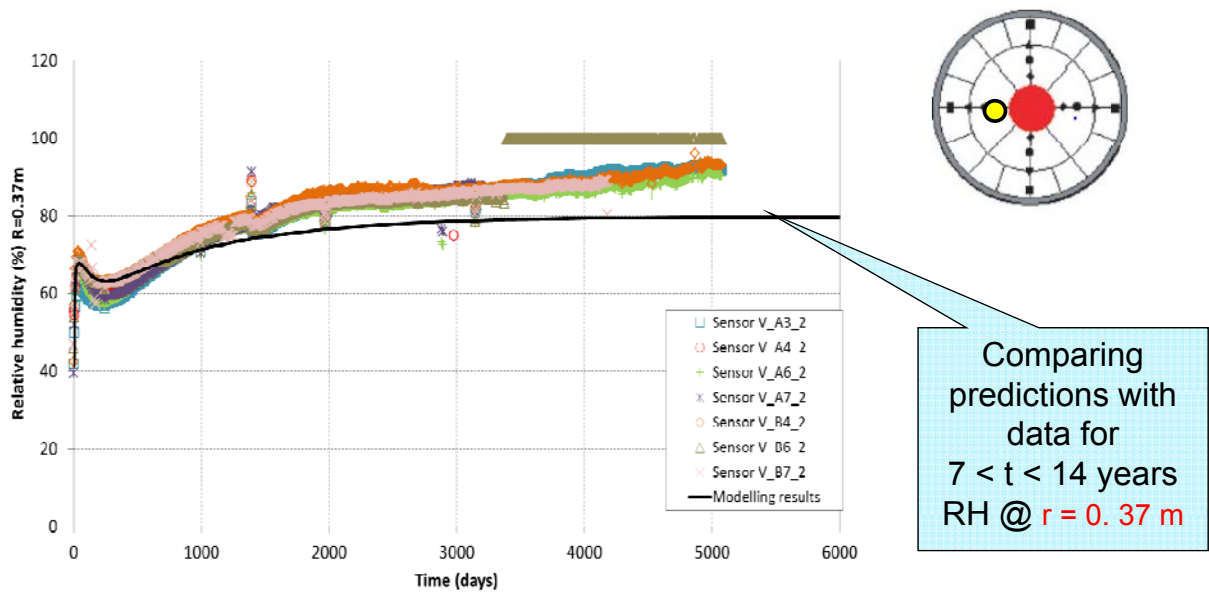
Extend the THC(m) model of the FEBEX mock up test from 7 to 14 years



Comparing predictions with data for $7 < t < 14$ years
RH @ $r = 0.55$ m

THMC model testing: mock-up test

Extend the THC(m) model of the FEBEX mock up test from 7 to 14 years



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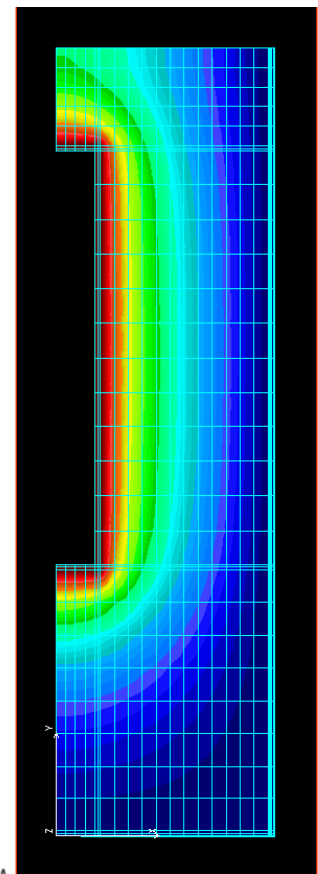
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THMC model testing: mock-up test

- Water uptake data are well predicted
- Discrepancies in relative humidity in the inner part could be due to model limitations
 - 2D axisymmetric versus 3D axisymmetric model which accounts for hot and dry areas
 - Single versus dual porosity for bentonite
 - Overheating episode



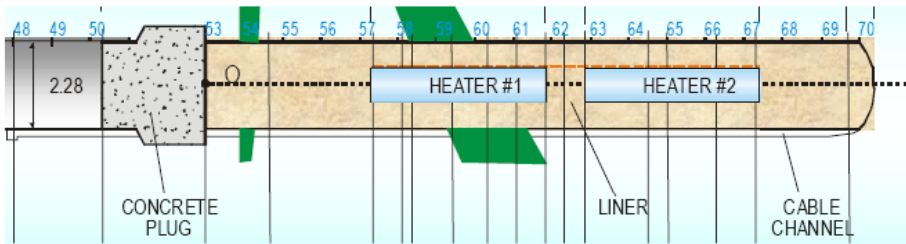
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THMC model testing: in situ test



Installation (1997)



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Dismantling (2002)

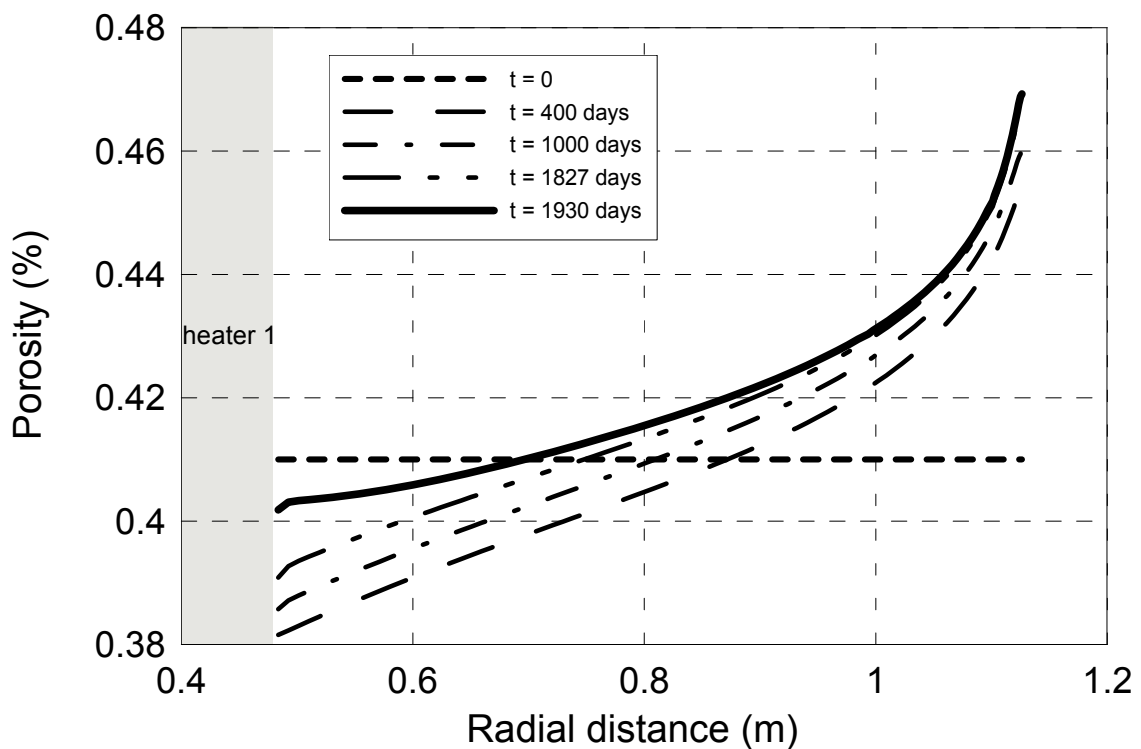


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THMC model testing: in situ test

Time evolution of porosity



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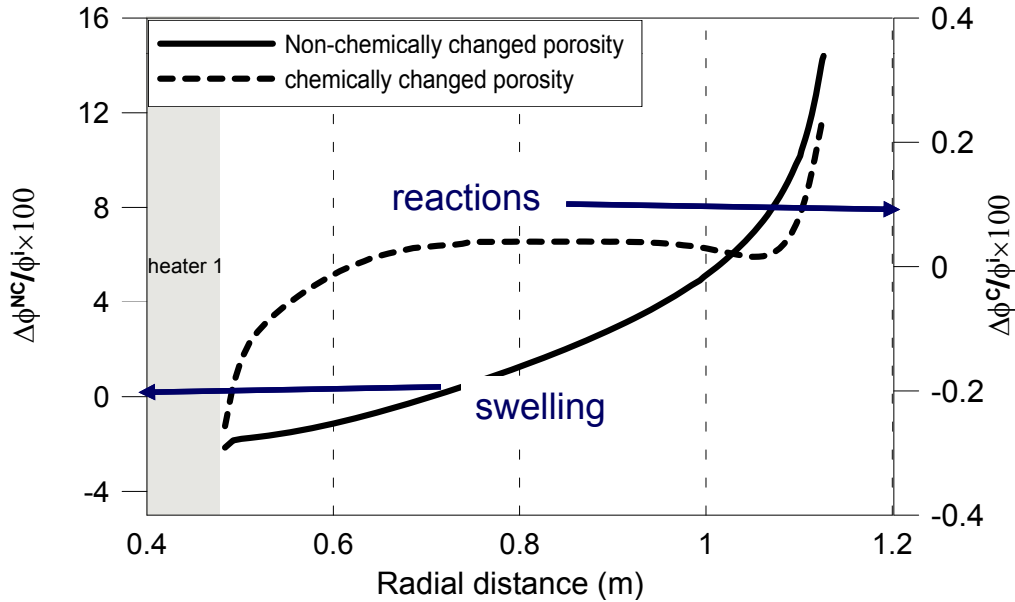
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THMC model testing: in situ test

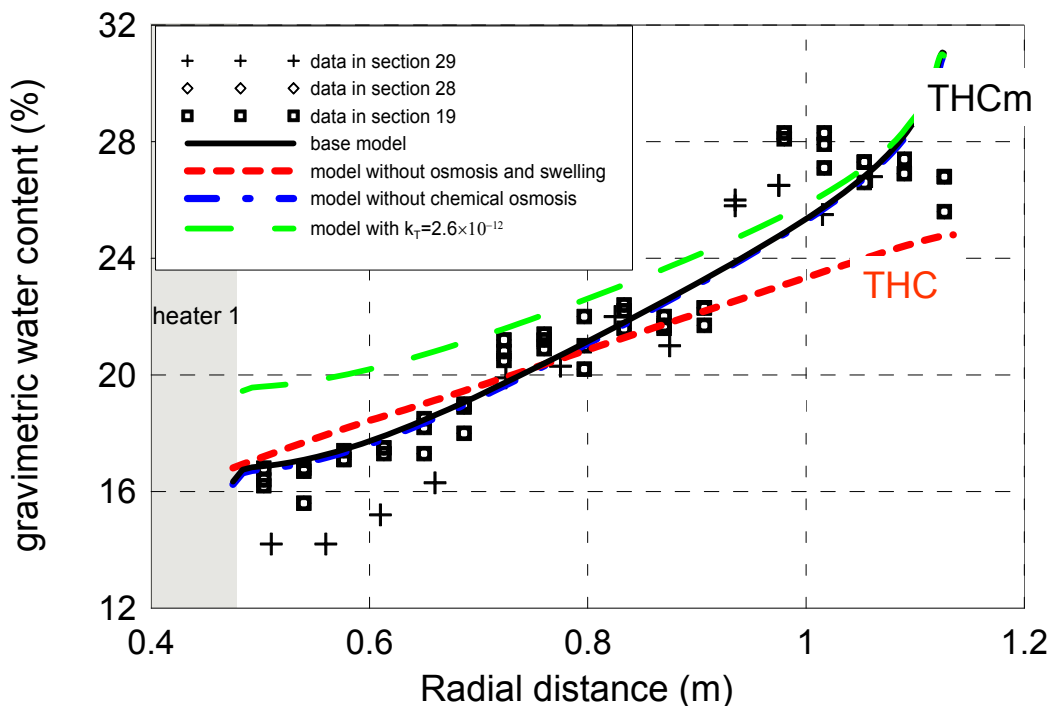
Mechanisms for porosity change

- Swelling (NC)
- Mineral dissolution/precipitation (C)



THMC model testing: in situ test

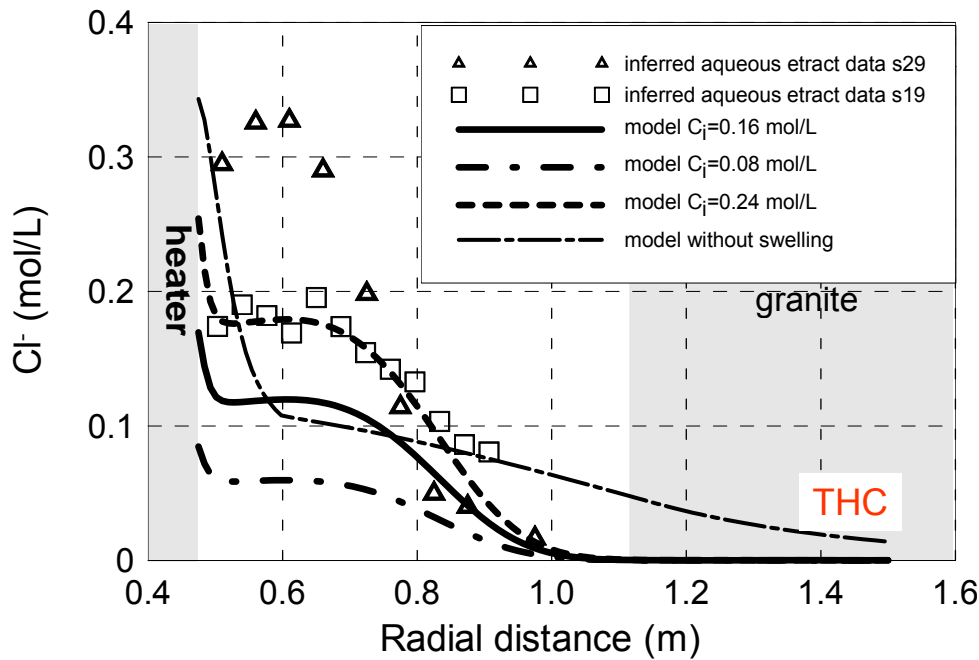
Water content data



THMC model testing: in situ test

Chemical data: Cl

- THC versus THCM model
- Sensitive to initial concentrations



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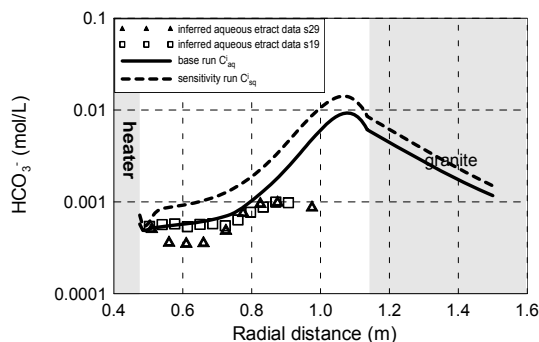
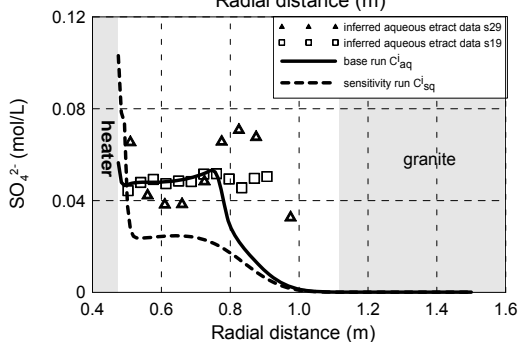
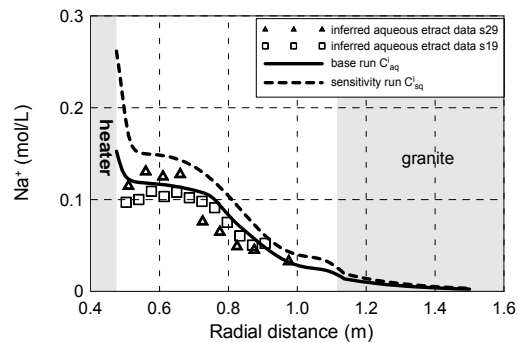
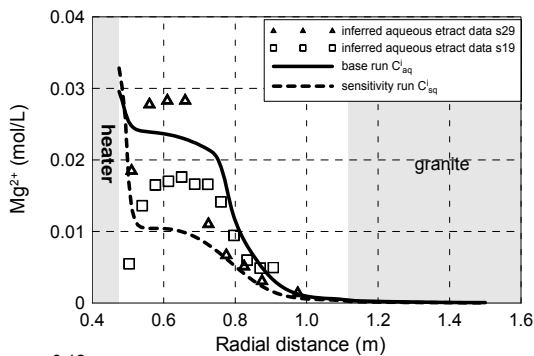
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THMC model testing: in situ test

Chemical data: Mg, Na, sulfate, bicarbonate

- Sensitive to initial concentrations



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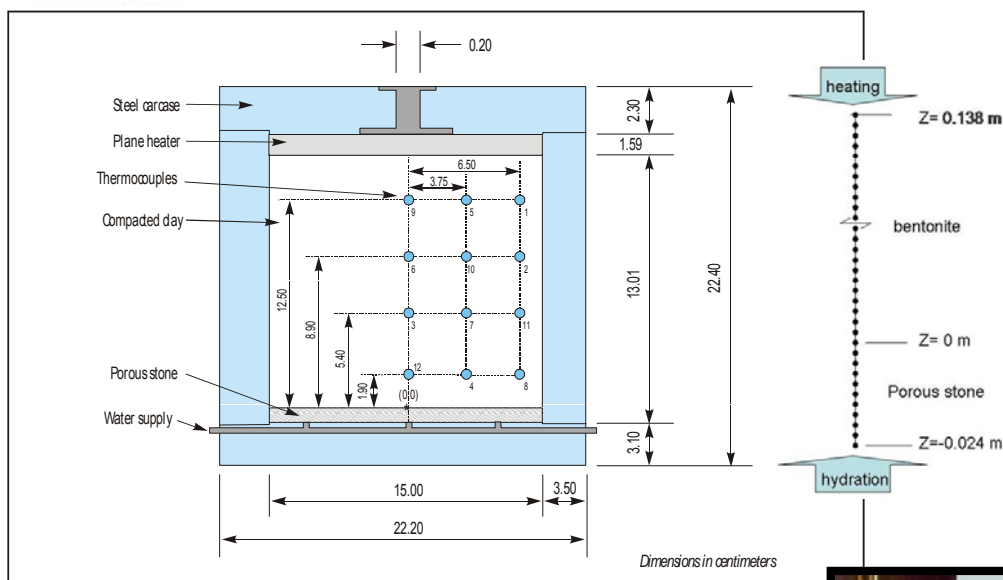
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THMC model testing: in situ test

- Chemical osmosis is not relevant
- Water contents are sensitive to thermal osmosis
- Computed concentrations deviate from measured data at the heater–bentonite and bentonite–granite interfaces because the model fails to account properly for the volume change of bentonite

THMC model testing: CT test



(Zheng et al., 2010; J Hydrol)



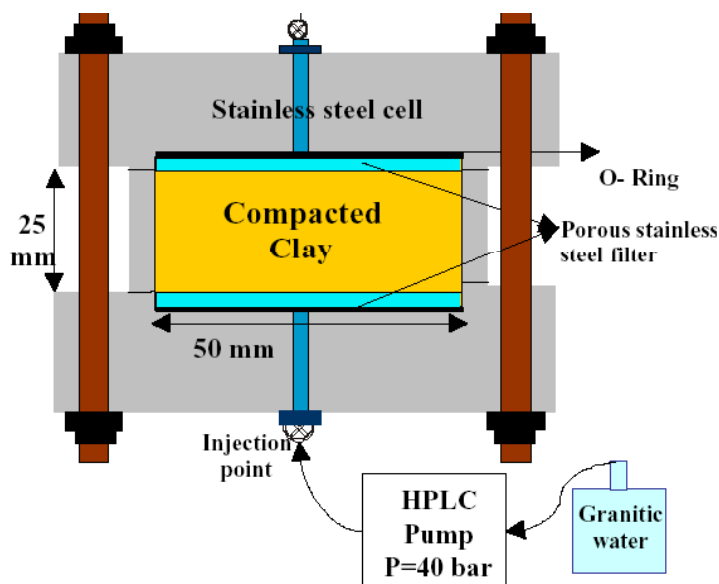
THMC model testing: CT test

- Changes in porosity due to swelling are important
- Changes in the spatial distribution of temperatures affect:
 - The evaporation/condensation pattern
 - Concentration of chemical species
- Water content is sensitive to thermal osmosis
- pH is buffered by surface protonation/deprotonation
- There are uncertainties in
 - The initial chemical composition of the bentonite porewater
 - The initial amount of sulphate minerals

THMC model testing: dual porosity

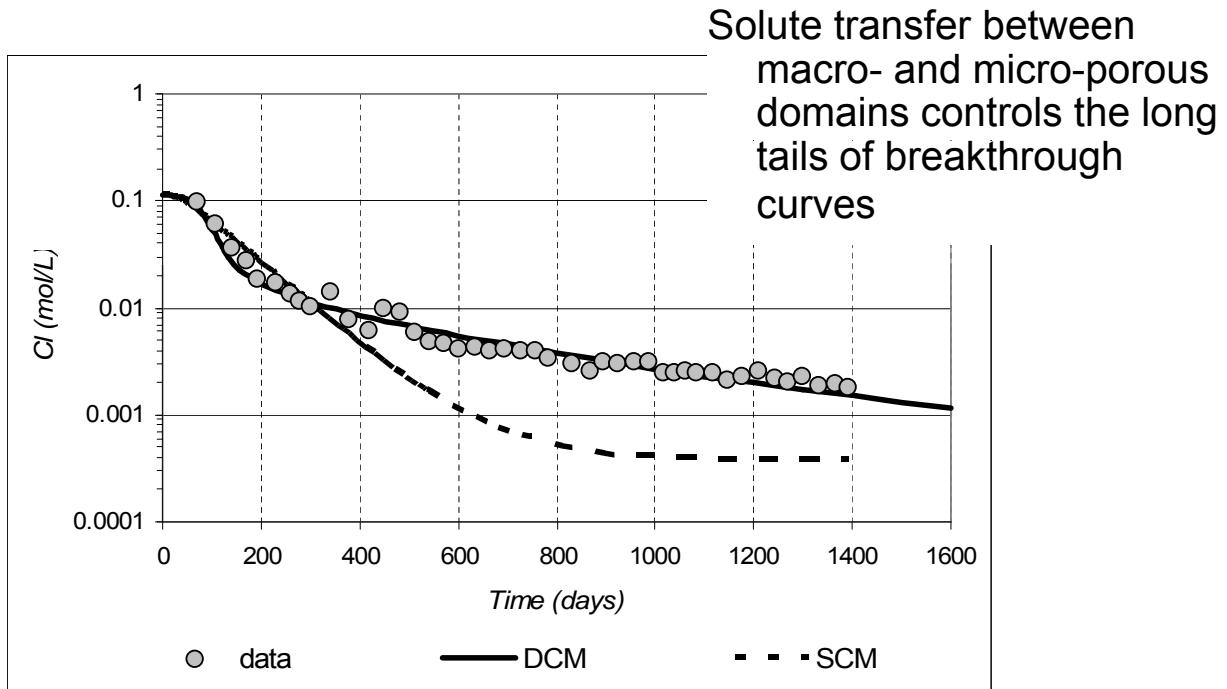
Permeation test

- Long tails of breakthrough curves
- Dual and single continuum models: DCM & SCM



THMC model testing: dual porosity

Cl⁻ breakthrough curves for single & dual porosity models



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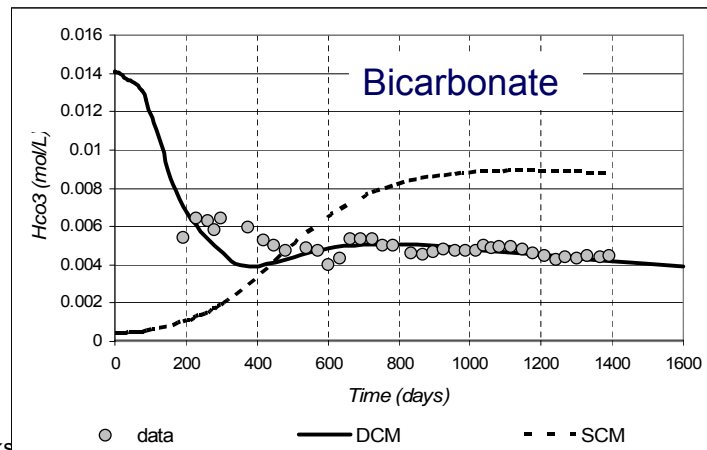
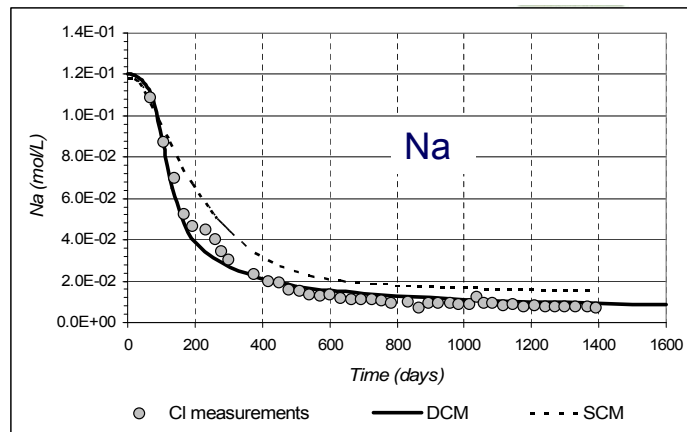
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THMC model testing: dual porosity

- DCM outperforms SCM
- Difficulties in parameterization are overcome by
 - Relying on a comprehensive clay characterization of FEBEX bentonite
 - Inverse estimation



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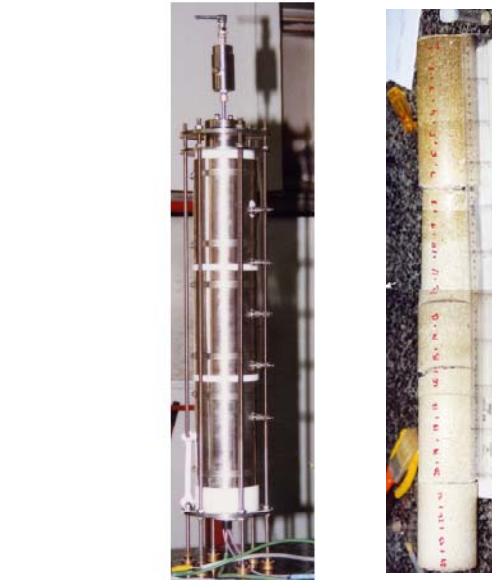
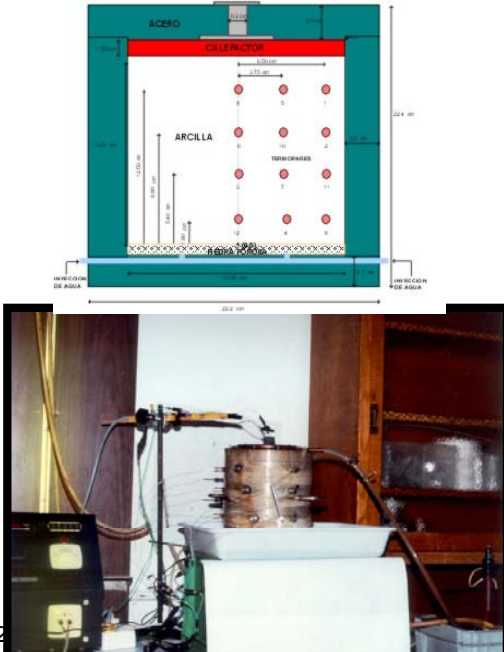
Regulatory Authority Works

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- Integrated analysis of laboratory and in situ tests at different space and time scales

CT CELLS ($L = 0.12\text{ m}$)

CG CELLS ($L = 0.60\text{ m}$)



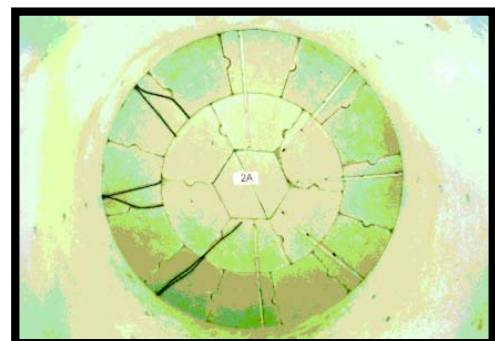
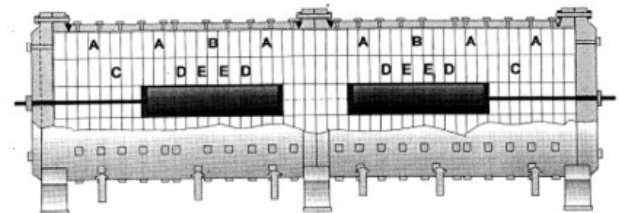
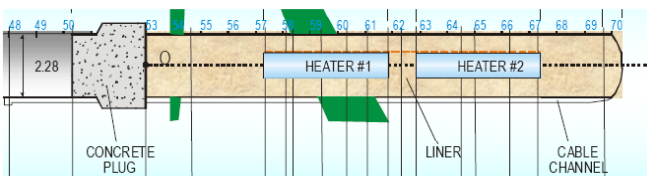
April 2

hop

- Integrated analysis of laboratory and in situ tests at different space and time scales

IN SITU TEST ($R = 0.6$)

MOCK-UP TEST ($R = 0.6$)



Apr

kshop

- Methodology
 - Revise and filter data
 - Transform in dimensionless variables

Time

$$t_D = \frac{K}{\rho g \alpha L^2} t$$

Distance

$$r_D = \frac{r_i}{L}$$

Time

$$t_D = \frac{K}{\rho g \alpha L^2} t$$

Water uptake

$$V_D = \frac{4V}{\pi D^2 L \Delta \theta}$$

Water content

$$\theta_D = \frac{\theta - \theta_i}{\theta_{sat} - \theta_i}$$

Temperature

$$T_D = \frac{T - T_b}{T_h - T_b}$$

Concentration

$$c_D = \frac{c - c_b}{c_i - c_b}$$

- r_D : dimensionless distance
- r_i : distance to the hydration boundary
- L : bentonite thickness
- K : hydraulic conductivity
- α : bentonite compressibility
- θ_D : dimensionless water content
- θ_i : initial water content
- θ_{sat} : saturated water content
- T_D : dimensionless temperature
- T_b : temperature in the hydration boundary
- T_h : temperature in the heater boundary
- c_D : dimensionless concentration
- c_b : concentration in the hydration boundary
- c_i : concentration in the bentonite

- Methodology
 - Revise and filter data
 - Transform in dimensionless variables

Concentration

$$c_D = \frac{c - c_b}{c_i - c_b}$$

Distance

$$r_D = \frac{r_i}{L}$$

Time

$$t_D = \frac{K}{\rho g \alpha L^2} t$$

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Temperature

$$T_D = \frac{T - T_b}{T_h - T_b}$$

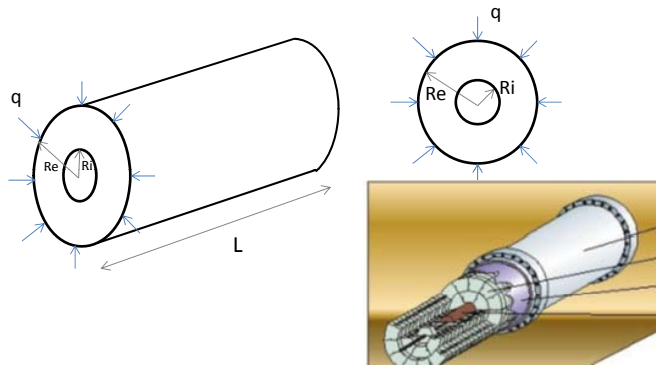
Concentration

$$c_D = \frac{c - c_b}{c_i - c_b}$$

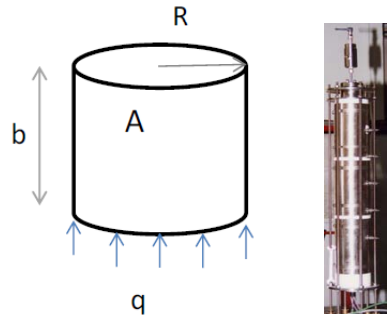
- r_D : dimensionless distance
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- T_b : temperature in the hydration boundary
- T_h : temperature in the heater boundary
- c_D : dimensionless concentration
- c_b : concentration in the hydration boundary
- c_i : concentration in the bentonite

- Water uptake: **dimensionless data**

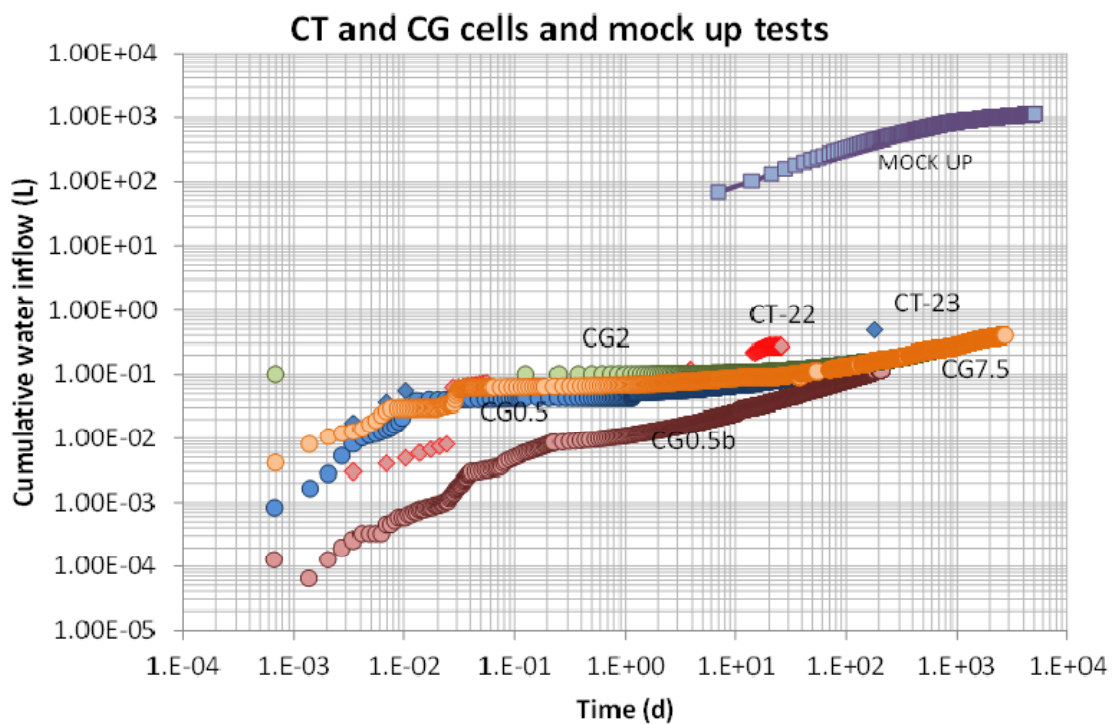
- Radial flow



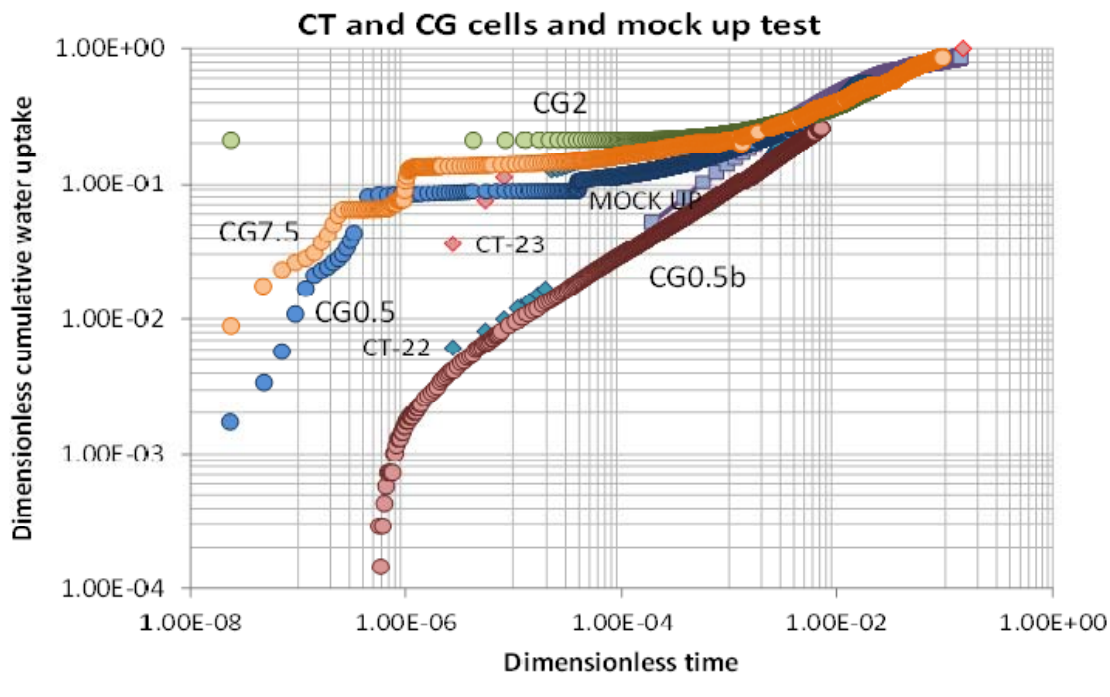
- Parallel flow



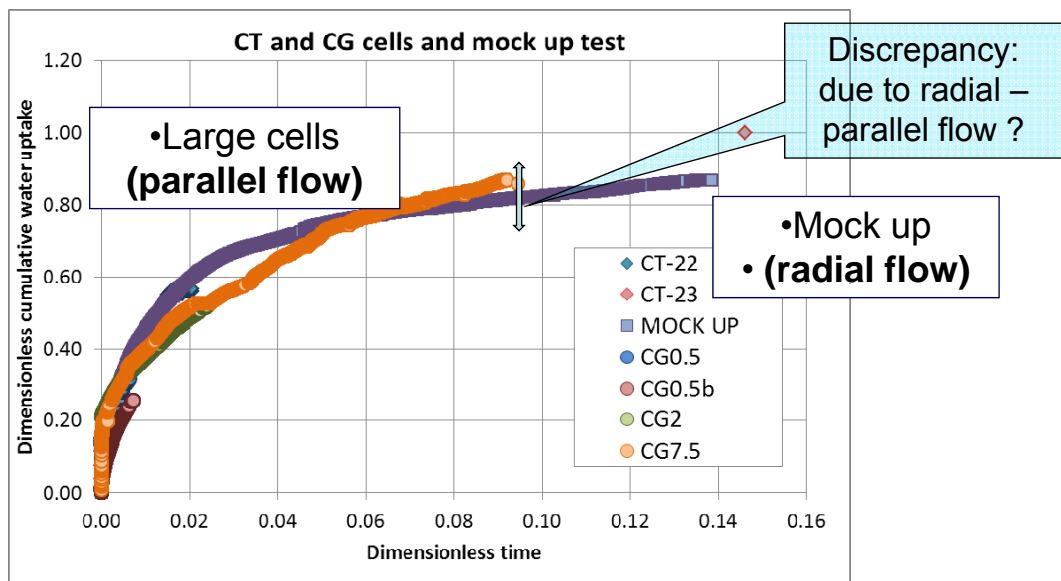
- Water uptake: **raw data**



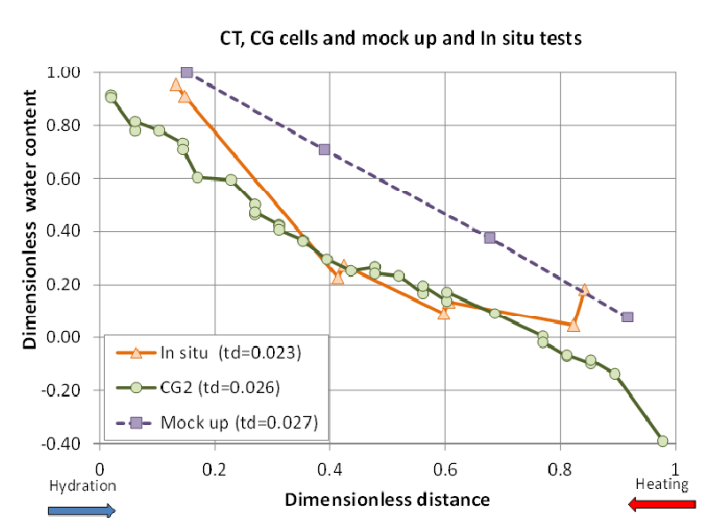
- Water uptake: dimensionless data



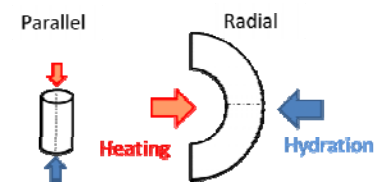
- Water uptake: dimensionless data



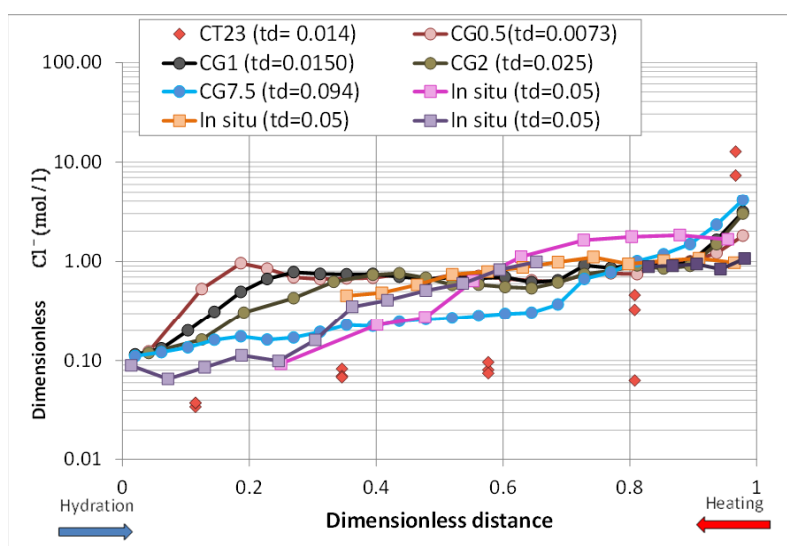
- Water content data



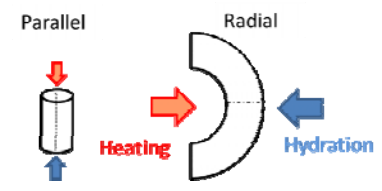
- Causes of differences:
 - Geometry
 - Initial flooding of the mock up test which induced a larger initial water content
 - Temperature gradients



- Chemical data: Cl⁻



- Causes of differences:
 - Geometry
 - Temperature gradients
 - Hydration water
 - Initial hydration of the mock up tests



Data from the different tests cannot be scaled-up due to differences in:

- Geometry
 - Radial
 - Parallel
- Method of bentonite hydration
- Temperature gradient
- Chemistry of hydration water

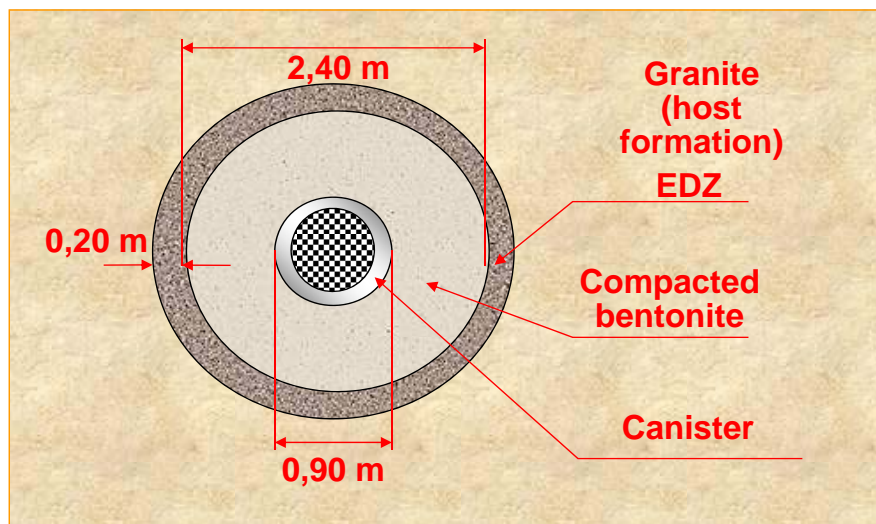
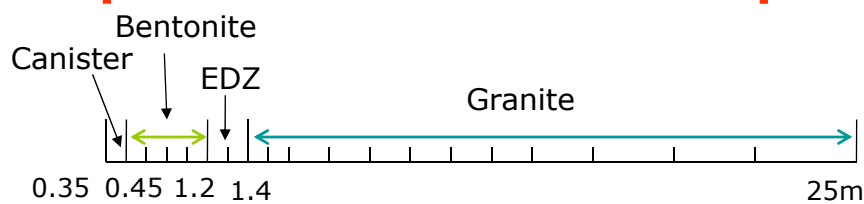
Natural Analogs

- Evaluation of natural analogues in terms of their usefulness for the validation of long-term extrapolation
 - Very few specific references to natural analogs studies have been found in PA studies
 - More frequent in the detailed documents supporting the main PA reports) and in general they have had a limited role in the overall evaluation of safety
 - Main uses of natural analogs in PA
 - Conceptual model development by providing useful information for the understanding of specific key processes
 - Model and geochemical database testing
 - Increasing confidence in extrapolating results from lab and field experiments to the repository
 - Natural analogs are not found to be well-defined in terms of boundary and initial conditions and model parameters.
 - Their use as a tool for long-term predictions in PEBS project is highly questionabl

SF REPOSITORY IN GRANITE

- Coupled thermal-hydrodynamic and geochemical calculations of mass balance and fluxes in the NF during and after the saturation phase
- Coupled modelling of canister corrosion and bentonite porewater interactions. Reactive diffusion of corrosion products.

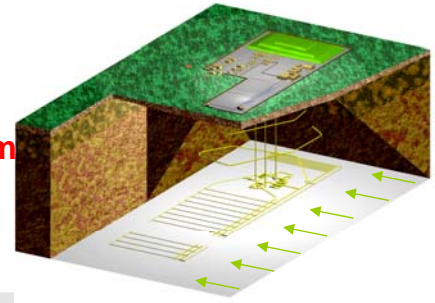
Spanish reference concept



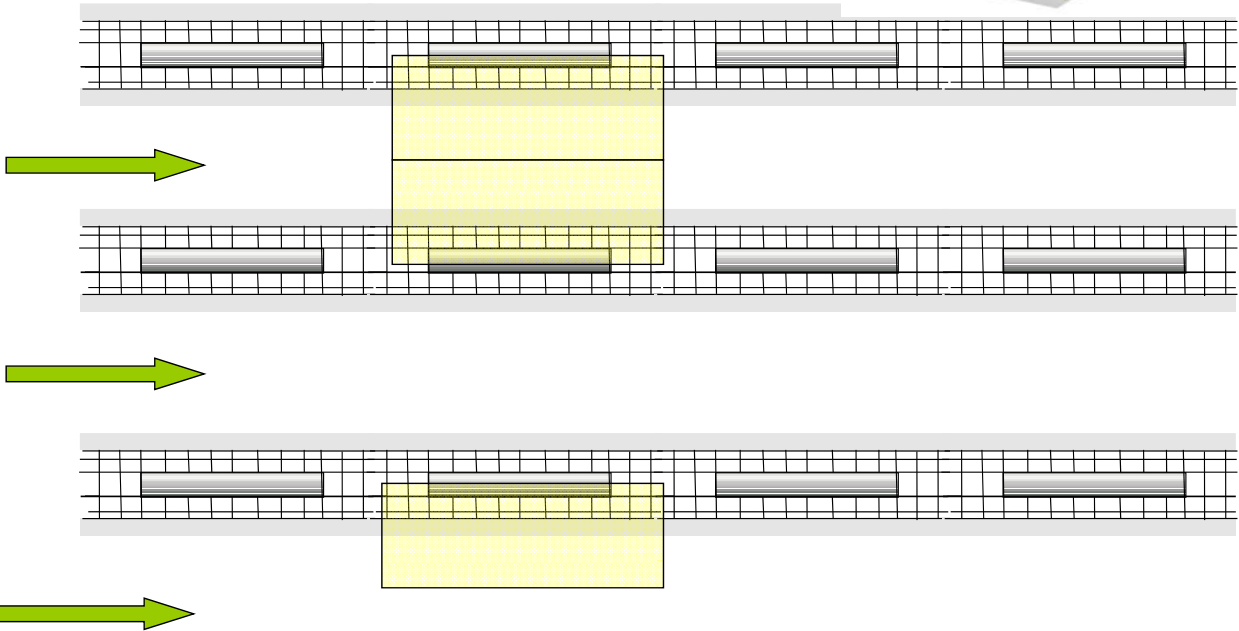
Disposal galleries

Conceptual model

Length 500 m
 Spacing gallery 50 m
 Spacing canisters 2,5 m



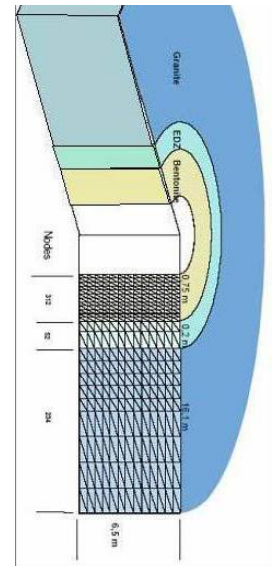
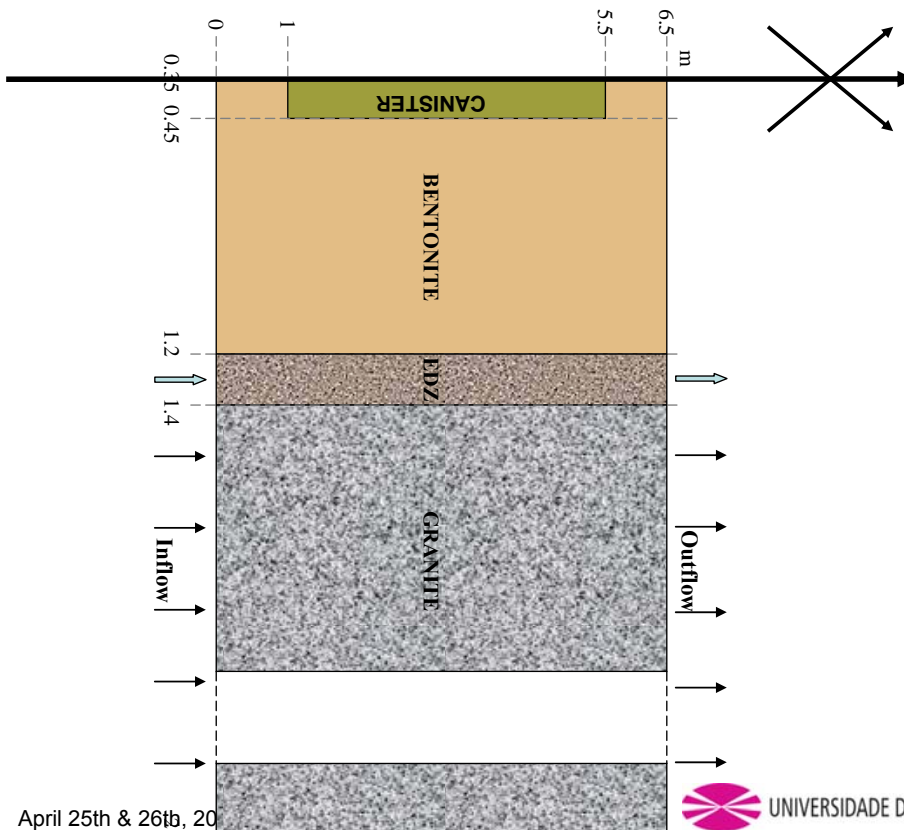
Water flow Total flow rate = 4.59 L/y per gallery



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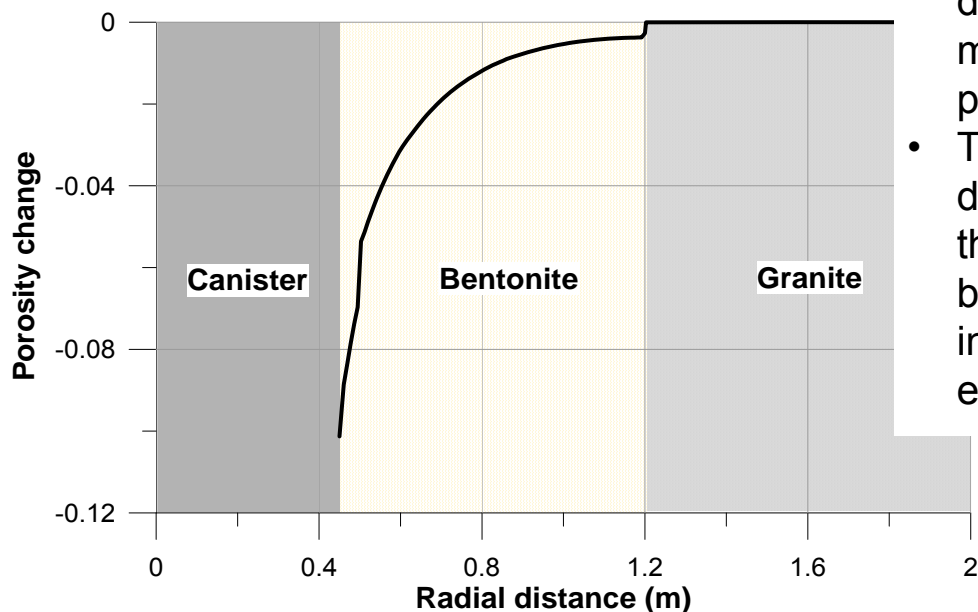
2D axisymmetric model



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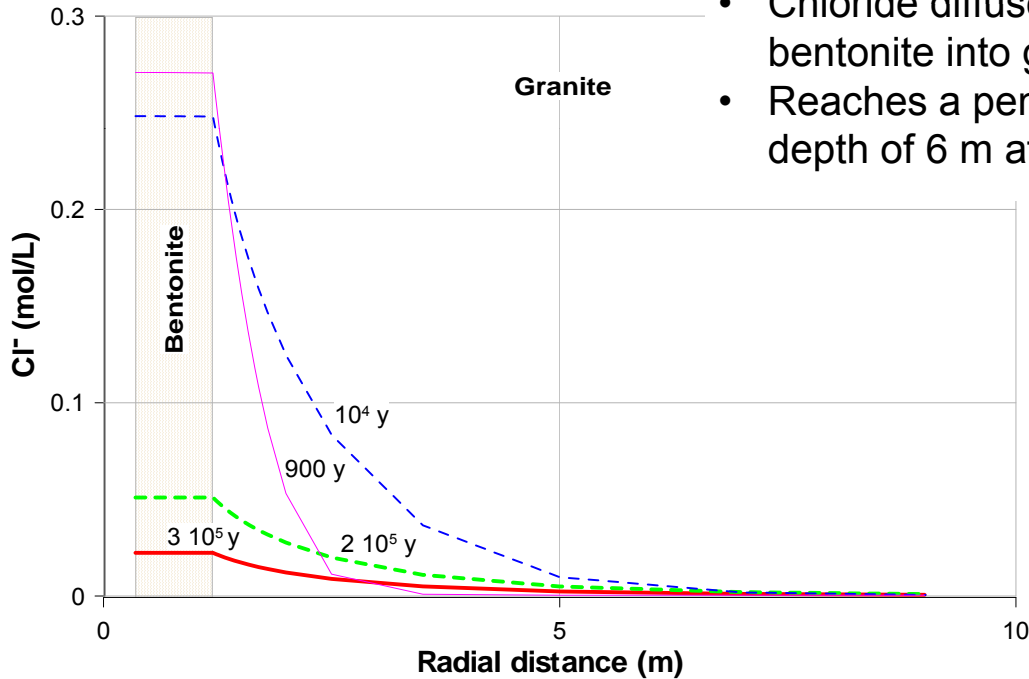
- Reactive transport model to predict the long term (during 300 000 years) hydrochemical evolution of the porewater composition in the near field of a repository in granite
 - Advection in granite, diffusion in bentonite
 - Multicomponent reactive transport
 - Chemical reactions
 - 12 components
 - 7 minerals
 - 5 exchange species
 - 4 Surface sorption species
- The model is isothermal and starts after bentonite has reached full water saturation
- Solve with CORE^{2D} V4 (Samper et al., 2009)

Spatial distribution of porosity changes at $t = 0.3$ Ma



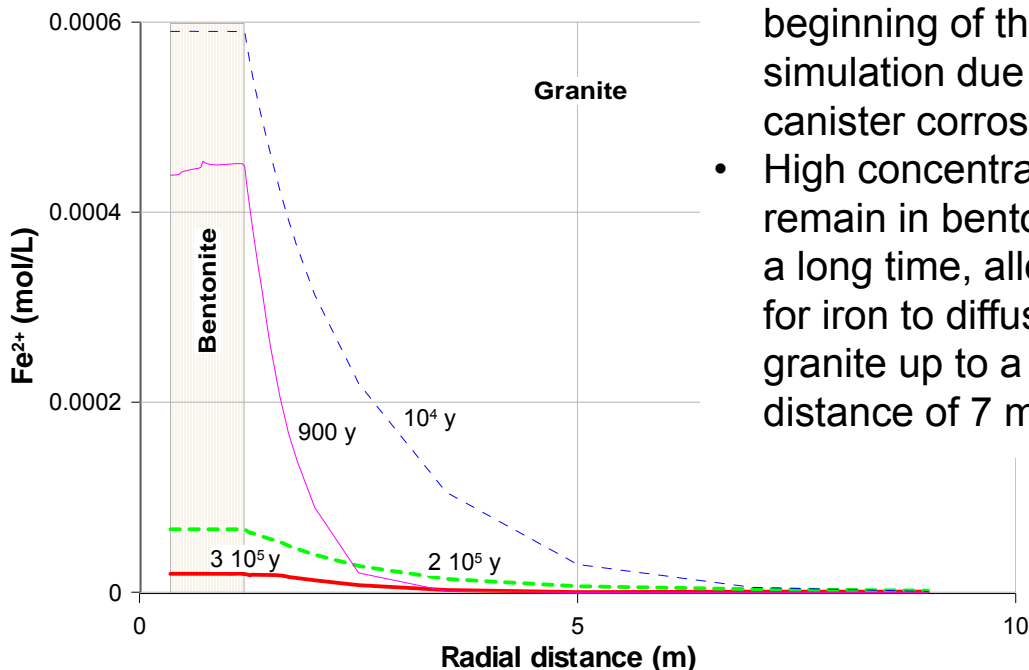
- Porosity in bentonite decreases due to magnetite precipitation
- The largest decrease is at the canister–bentonite interface and is equal to 0.1

Spatial distribution of Cl⁻ at different times



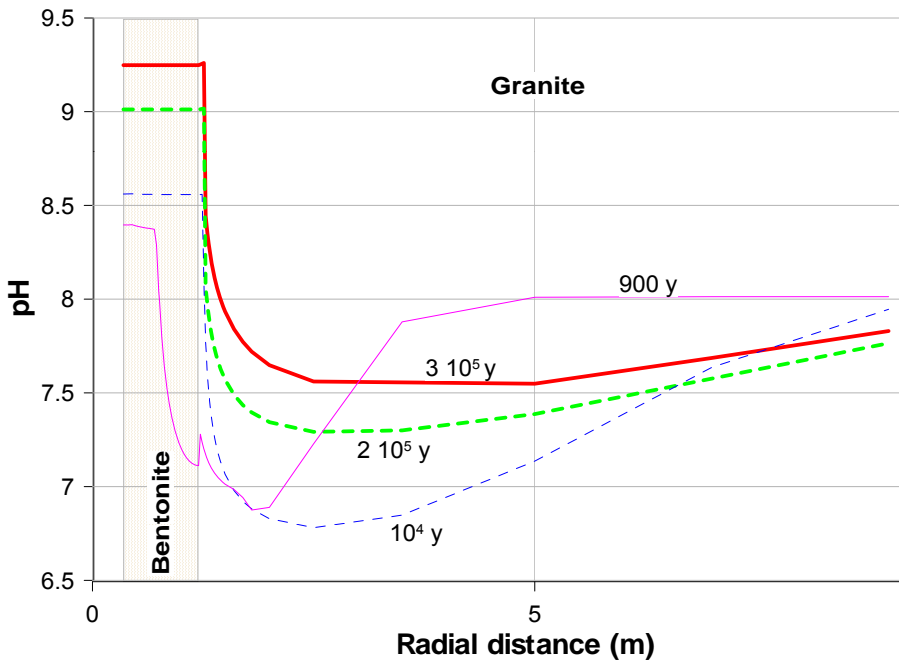
- Chloride diffuses from bentonite into granite
- Reaches a penetration depth of 6 m after 0.3 Ma

Spatial distribution of Fe at different times



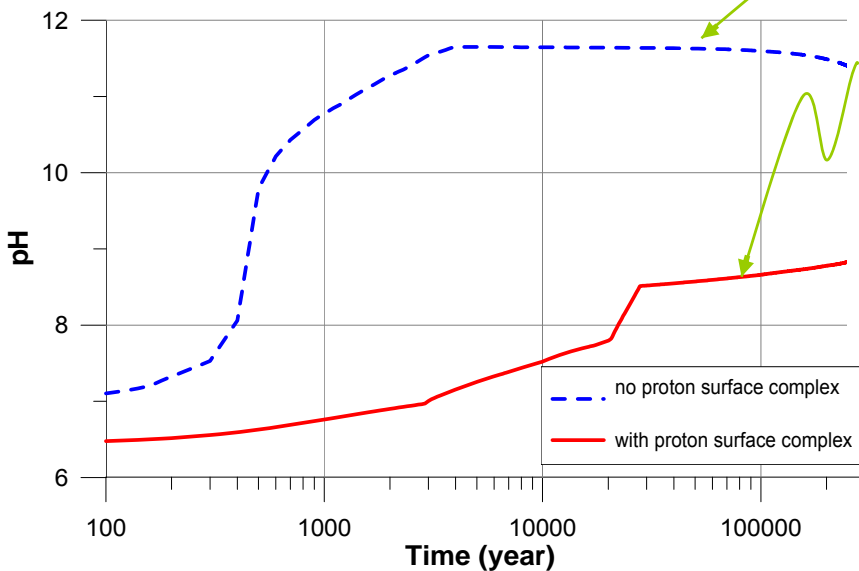
- Fe in bentonite and granite increase at the beginning of the simulation due to canister corrosion
- High concentrations remain in bentonite for a long time, allowing for iron to diffuse into granite up to a radial distance of 7 m.

Spatial distribution of pH at different times



- Initial pH in granite (8.0) is larger than that in bentonite (6.4)
- Initially, protons diffuse from bentonite into granite
- Later, corrosion causes a steady increase of pH in bentonite.
- The largest pH in bentonite is 9.25 after 0.3 Ma

pH in bentonite: sensitivity to surface complexation



- A high pH of almost 12 is calculated when proton surface complexation is ignored
- pH remains below 9 due to proton surface complexation
- Proton surface complexation is highly effective in buffering pH of bentonite

- A significant progress on THCM models for the EBS has been achieved
- Bentonite swelling & thermal osmosis are relevant for bentonite hydration and solute transport
- Model improvements & extensions
 - Bentonite-concrete & bentonite-canister interfaces
- Data from the different tests cannot be scaled-up due to differences in geometry, hydration conditions, temperature gradient and chemistry of hydration water

- The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement 232598
- Laboratory experiments and the mock up test used for THMC modeling were carried out by CIEMAT (Madrid, Spain).

Authors: Javier Samper,
Luis Montenegro, Alba Mon, Acacia Naves,
Bruno Pisani

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Work Package 3

“Coupled thermo-hydro-mechanical modelling of the bentonite buffer”

Antonio Gens & Benoit Garitte, CIMNE



26 April 2012

PEBS Workshop

Saint Ursanne, Switzerland

Outline

- ❑ Objectives
- ❑ THM modelling: HE-E test
- ❑ Incorporation of new features and some modelling results
 - Double structure model
 - Threshold gradient
 - Thermo-osmosis
 - Osmotic/flow – chemistry coupling
 - Water density

- ❑ Objectives
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 - Water density

WP3 (start date: 1/3/2010)

Objectives

The overall objectives of this Work Package are

- to perform coupled HM, THM, and THMC analyses to provide a sound basis for the interpretation of the various tests planned in the frame of the PEBS WP2,
- to develop new or improved models as demanded by the calibration of computation results with the actual measured data, and
- to use the data and improved models for extrapolation to long-term evolution of the repository taking into account the scenarios defined in PEBS WP1 and to investigate model uncertainty and its impact on long-term prediction, thus providing input to PEBS WP4.

Description of work

All the process level modeling work is included in WP3. The Work Package is structured into five different tasks:

- Task 3.1: HM modeling of the Mont Terri Engineered Barrier (EB) Experiment
- Task 3.2: THM modeling for the planned heater test HE-E
- Task 3.3: THM modeling of bentonite buffer
- Task 3.4: Modeling of THM-C experiments on bentonite buffer
- Task 3.5: Extrapolation to repository long term evolution

The specific objectives and work descriptions are described in the respective task descriptions 3.1 –3.5.

- ❑ Objective: HM modelling of the Mont Terri Engineered Barrier (EB) Experiment
- ❑ The HM modelling will aim at providing a satisfactory scientific representation and a sound basis for interpretation of
 - The EB hydration phase (2D)
 - The final state of the barrier including dismantling effects (comparison with dismantling observations)

| Deliverables | | | |
|-----------------|---|------------------------|--------------------|
| Deliverable no. | Description/Deliverable name | Organisation in charge | Date of completion |
| D3.1-1 | Modeling and interpretation of the EB experiment hydration | ENRESA/CIMNE | Month 36 |
| D3.1-2 | D3.1-2 Interpretation of the final state of the EB experiment barrier | ENRESA/CIMNE | Month 45 |

- ❑ Objective: THM modelling of the planned heater test HE-E
- ❑ THM modelling will focus on:
 - Scoping calculations for the design of the HE-E test
 - Predictive modelling of the HE-E
 - Development/validation of constitutive models and selection of parameters for the EB materials and the Opalinus clay
 - Interpretative modelling of the HE-E test

| Deliverables | | | |
|-----------------|---|-----------------------------------|--------------------|
| Deliverable no. | Description/Deliverable name | Organisation in charge | Date of completion |
| D3.2-1 | Design and predictive modeling of the HE-E test | NAGRA/ TK Consult CIMNE/GRS | month 18 |
| D3.2-2 | Modeling and interpretation of the HE-E test | NAGRA/ TK Consult CIMNE/GRS | month 36 |

Objective: THM modelling of the bentonite buffer

Tasks

- Long term THM modelling of the mock up test
- Long term THM modelling of CIEMAT cell tests
- Incorporation of new processes

| Deliverables | | | |
|-----------------|--|------------------------|--------------------|
| Deliverable no. | Description/Deliverable name | Organisation in charge | Date of completion |
| D3.3-1 | THM validation modeling of selected WP2 experiments | NAGRA/ TK Consult | month 36 |
| D3.3-2 | Report on the modeling with initially available data | Clay Technology | month 18 |
| D3.3-3 | Modeling and interpretation of the FEBEX mock-up test and of the long-term THM tests | CIMNE | month 42 |

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Objective: Formulation of a model for long term predictions

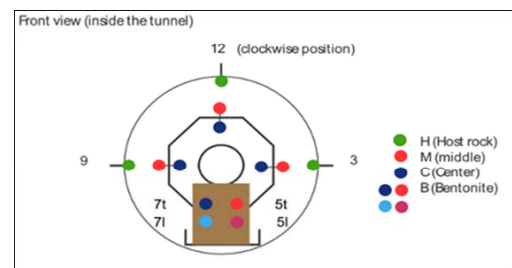
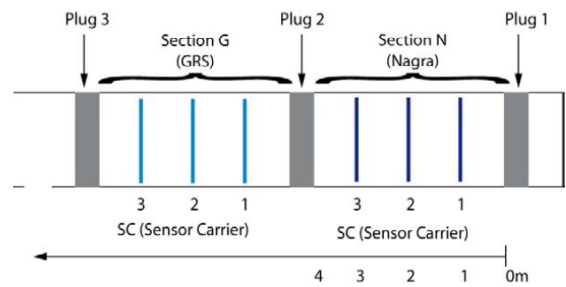
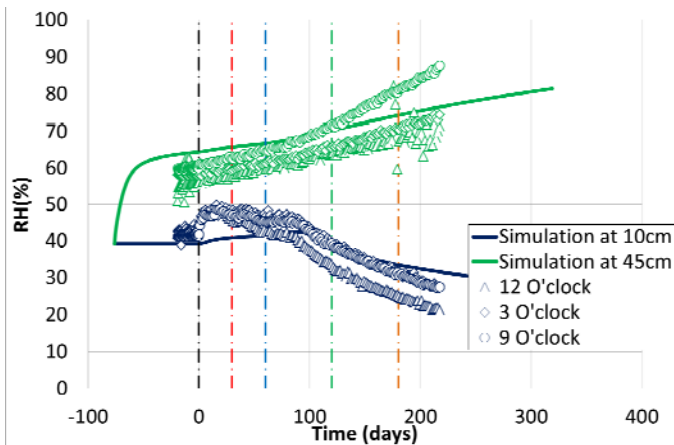
Features

- Double structure model
- Threshold gradient
- Thermo-osmosis
- Osmotic/flow – chemistry coupling
- Water density

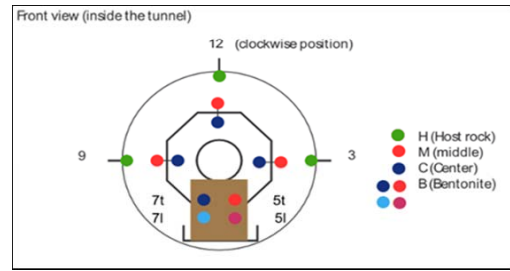
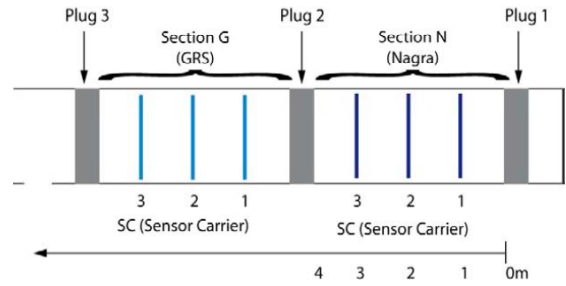
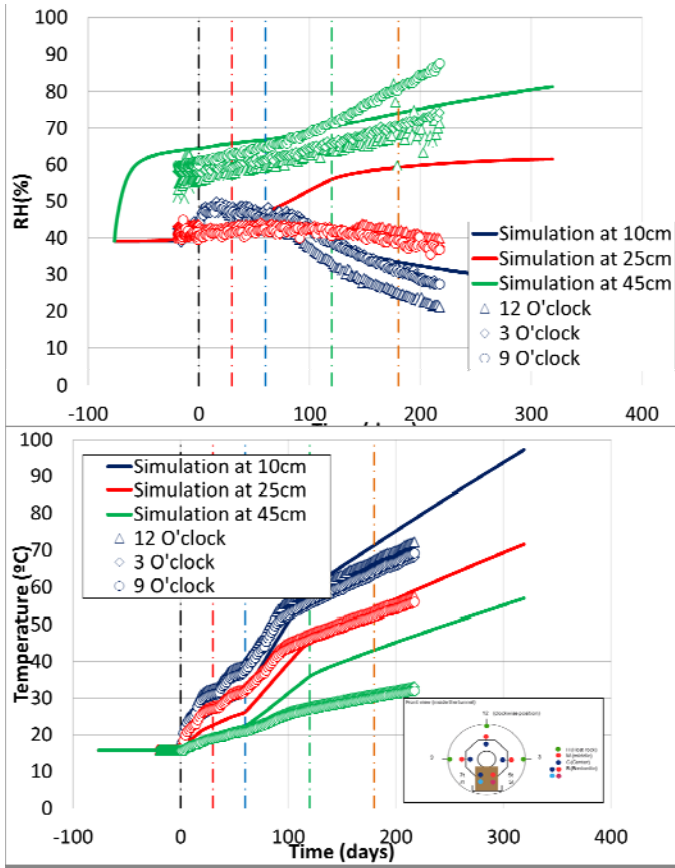
| Deliverables | | | |
|-----------------|--|------------------------|--------------------|
| Deliverable no. | Description/Deliverable name | Organisation in charge | Date of completion |
| D3.5-1 | Report on integration of available data for bentonites from different scales and scaling laws and extrapolation for long-term analyses for clay barriers | UDC | month 18 |
| D3.5-2 | Formulation of a model suitable for long term predictions | CIMNE | month 24 |
| D3.5-3 | Report on long-term THC(m) predictions of a HLW repository in granite | UDC | month 30 |
| D3.5-4 | Extrapolation of the models developed to the repository long-term evolution and evaluation of uncertainties | GRS plus all | month 45 |

- ❑ Objectives
- ❑ THM modelling: HE-E test
- ❑ Incorporation of new features and some modelling results
 - Double structure model
 - Threshold gradient
 - Thermo-osmosis
 - Osmotic/flow – chemistry coupling
 - Water density

HE-E: predictive modelling



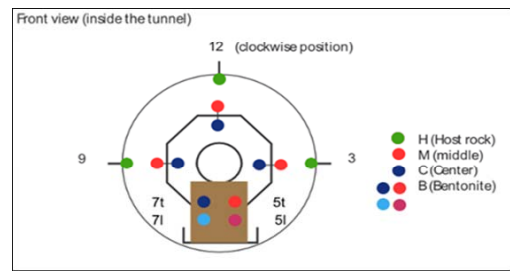
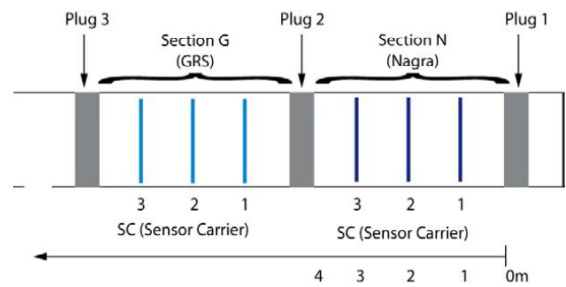
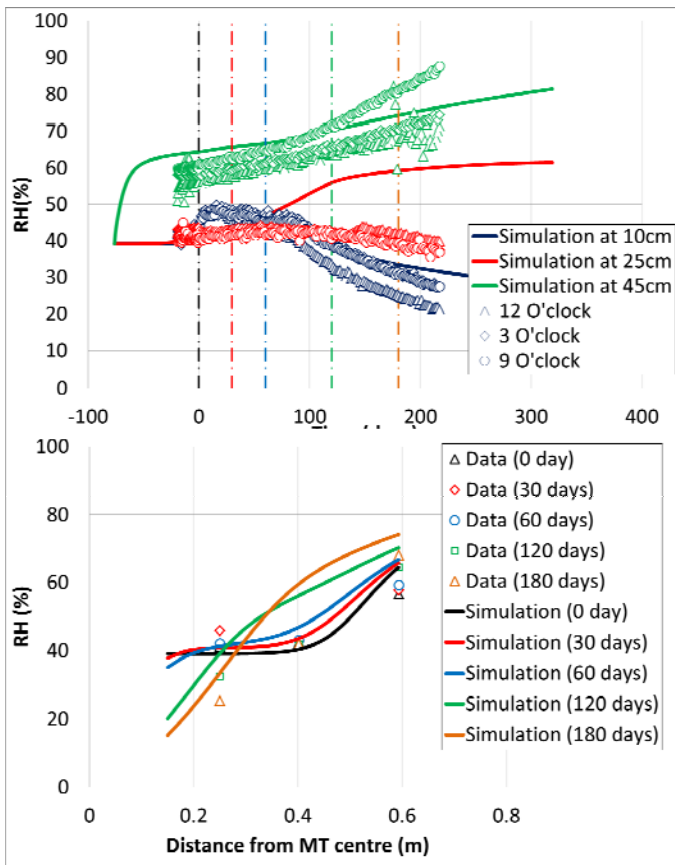
NAGRA N1



NAGRA N1

hop

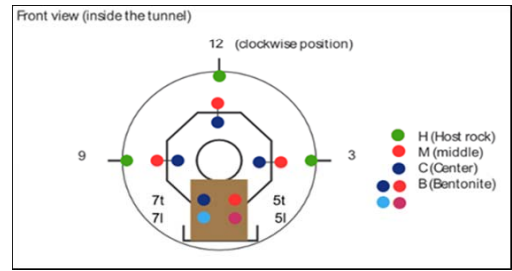
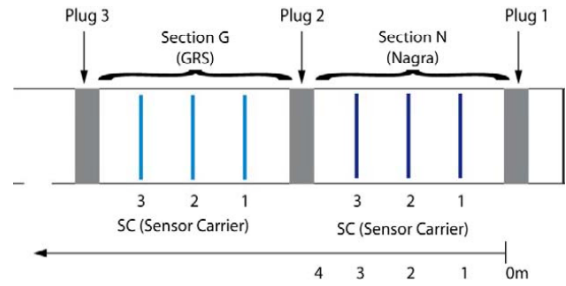
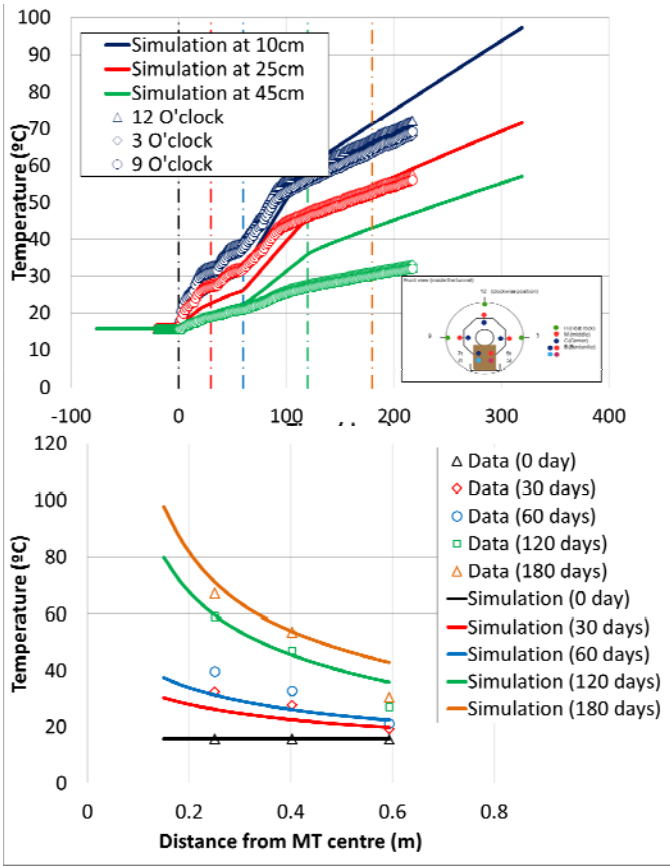
11



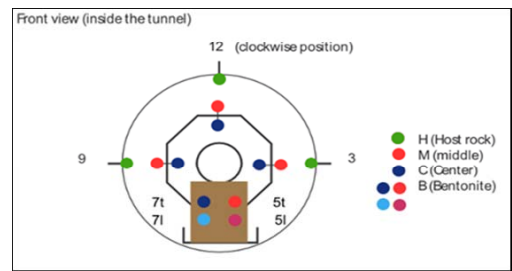
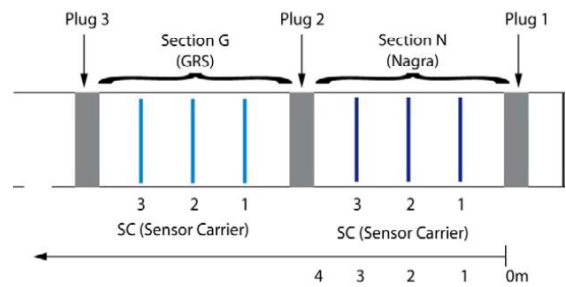
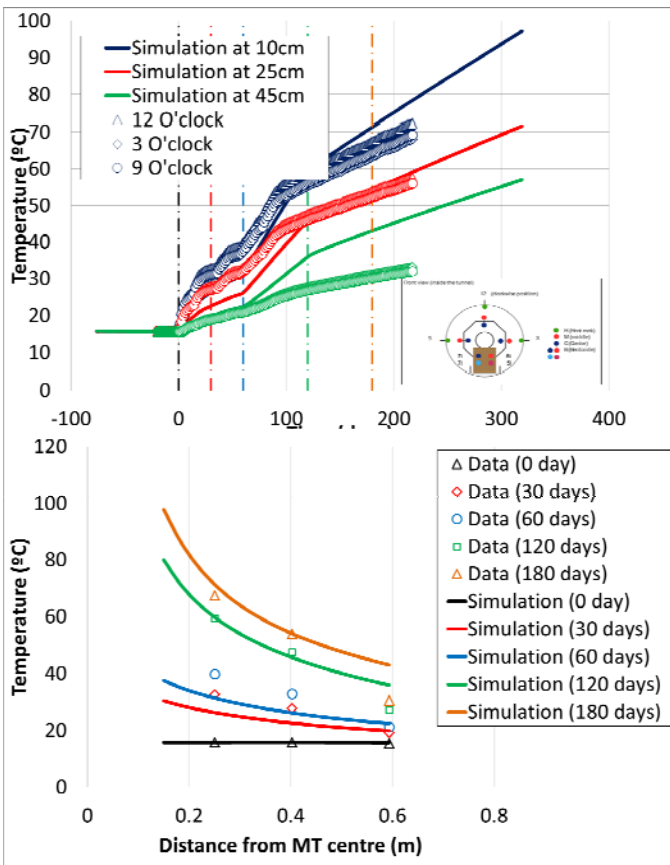
NAGRA N1

hop

12



NAGRA N1



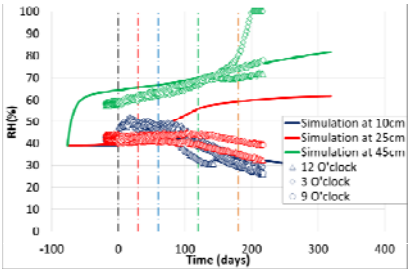
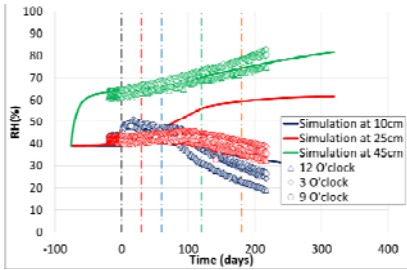
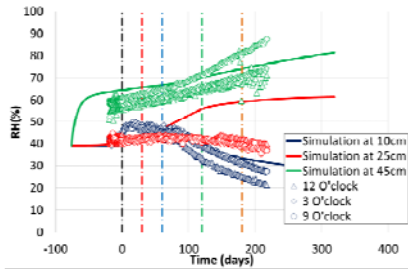
NAGRA N1

N1

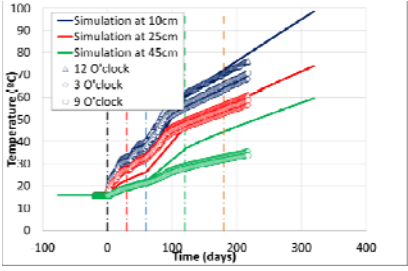
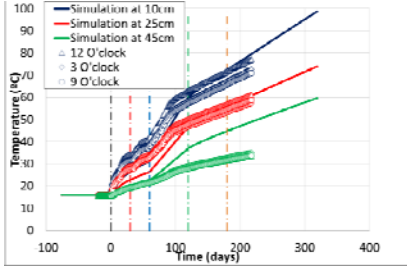
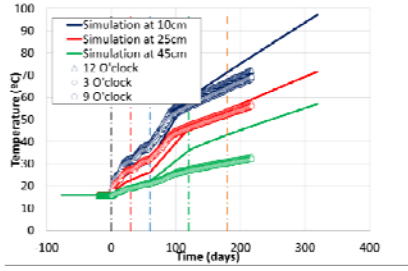
N2

N3

RH



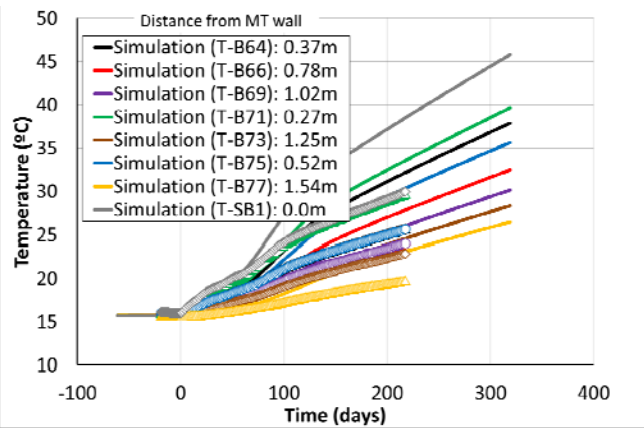
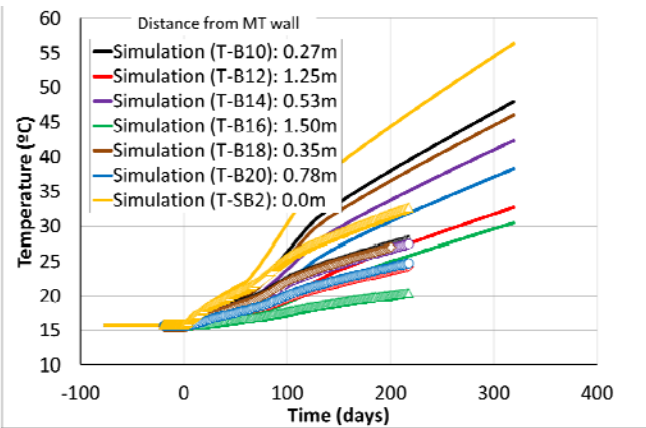
Temperature



NAGRA

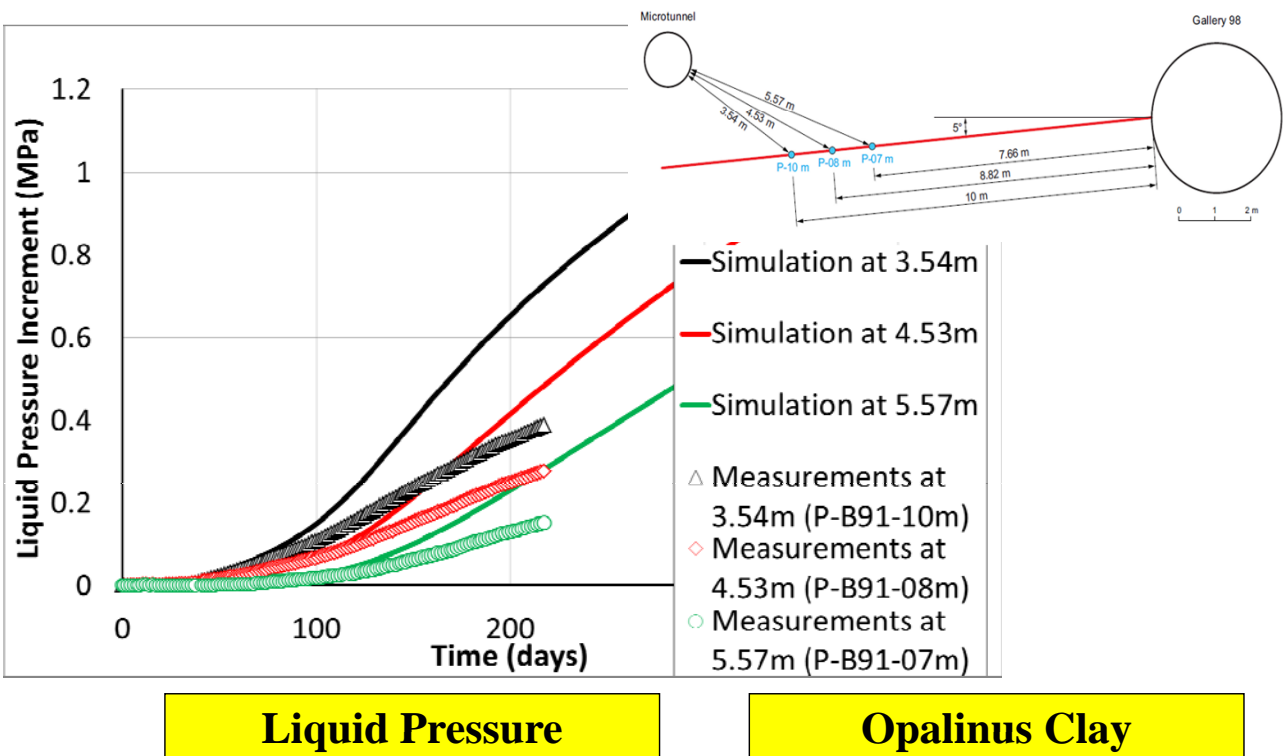
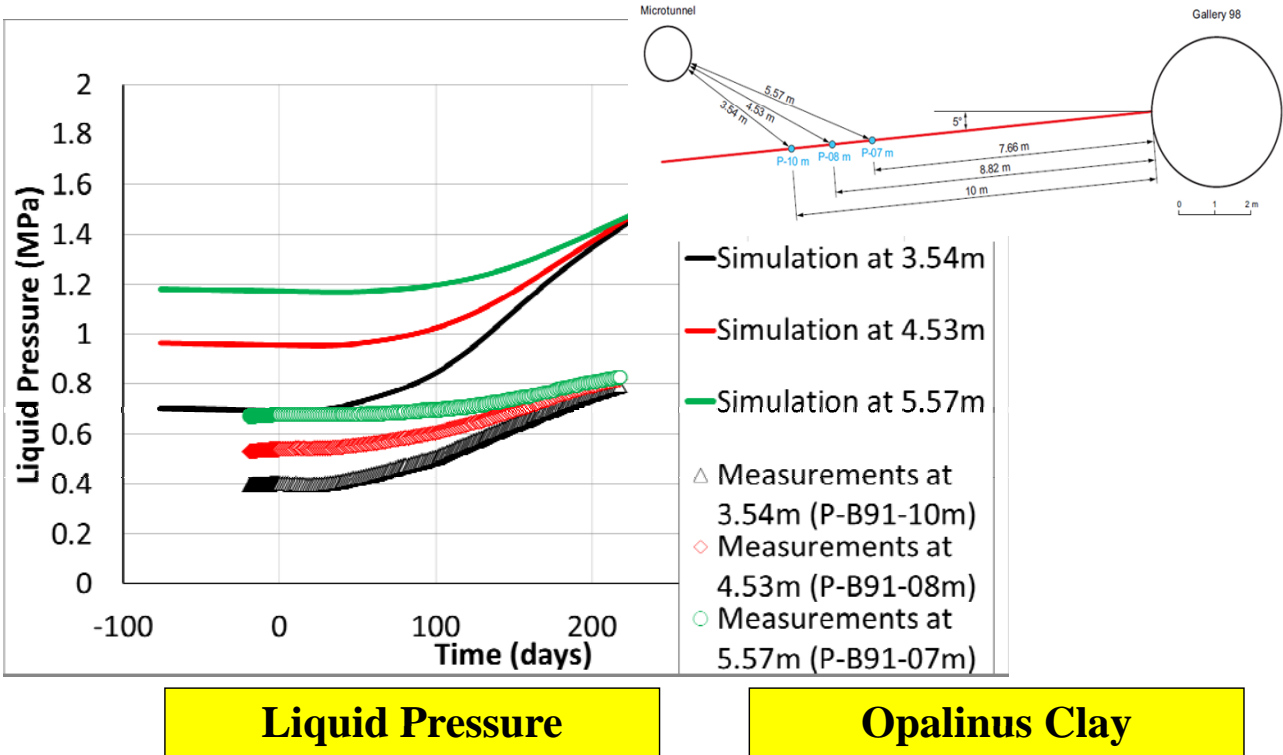
NAGRA

GRS



Temperature

Opalinus Clay



Intermediary remarks

- ❑ (Design) and predictive modelling were done with a basic model
- ❑ This simple model allows to get insights on on-going processes and is a useful tool to understand the set of measurements
- ❑ Two kinds of discrepancies between the model and the measurements are associated to:
 - Differences between the experiment geometry and the implemented boundary value problem
 - Inadequate/“not fully describing” constitutive laws for the material behaviour

Outline

- ❑ Objectives
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 - Osmotic/flow – chemistry coupling
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- ❑ Two structural levels are considered: macrostructure and microstructure

- ❑ The stress variables are:

- Net total stress:

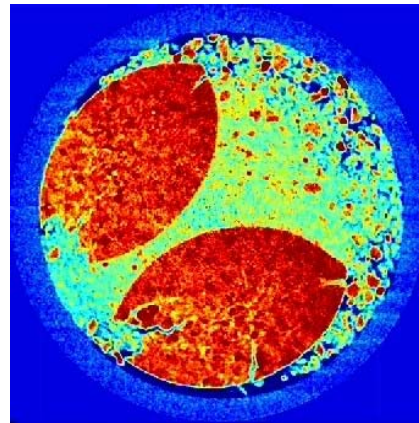
$$\sigma_{ij} - u_a \delta_{ij}$$

- Suction:

$$s = u_a - u_w \quad (\text{matric})$$

$$s_t = s + s_o$$

(total = matric + osmotic)



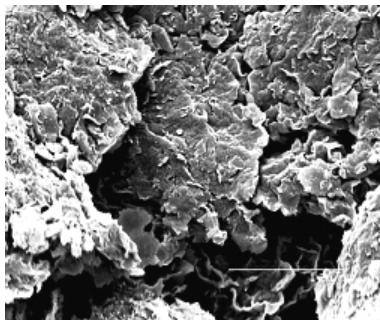
- Gens & Alonso (CGJ, 1992). Conceptual foundation
- Alonso, Vaunat & Gens (EG, 1999). First mathematical formulation
- Sánchez, Gens, Guimaraes & Olivella (IJNAMG, 2005). Formulation based on generalised plasticity
- Sánchez, Gens, Guimaraes & Olivella (C&G, 2008). Numerical implementation algorithms

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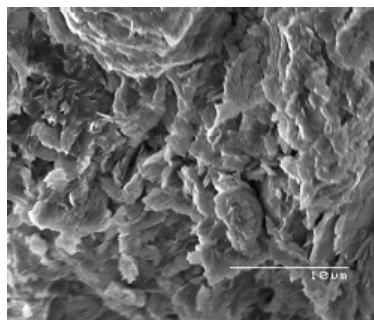
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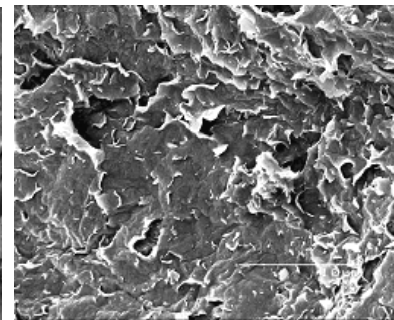
- ❑ Constitutive model for a double structure material: Evolution of the microfabric



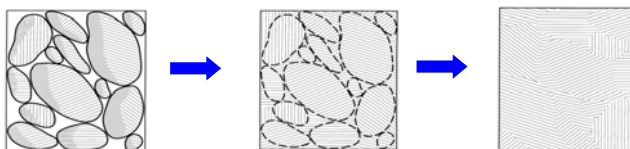
Compacted (suction ≈ 110 MPa)



Suction = 10 MPa



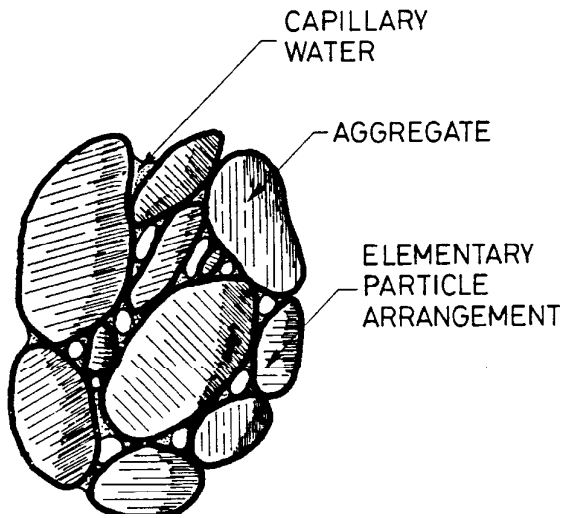
Saturated



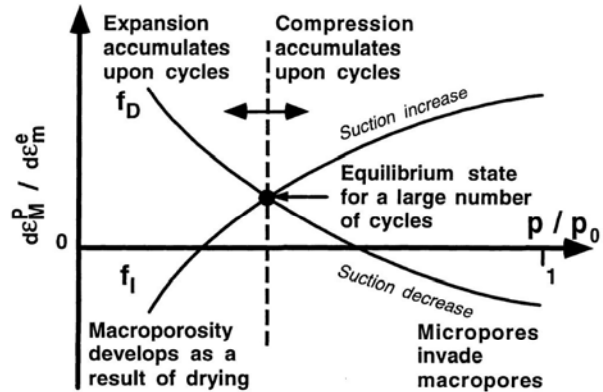
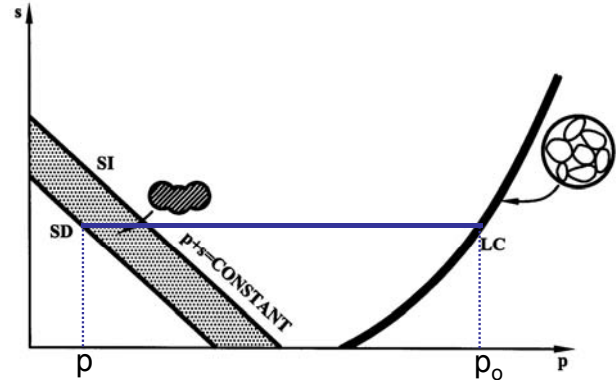
$$\phi = \phi_M + \phi_m$$

$$\mathbf{k} = \mathbf{k}(\phi_M)$$

- Constitutive model for a double structure material: Evolution of the microfabric



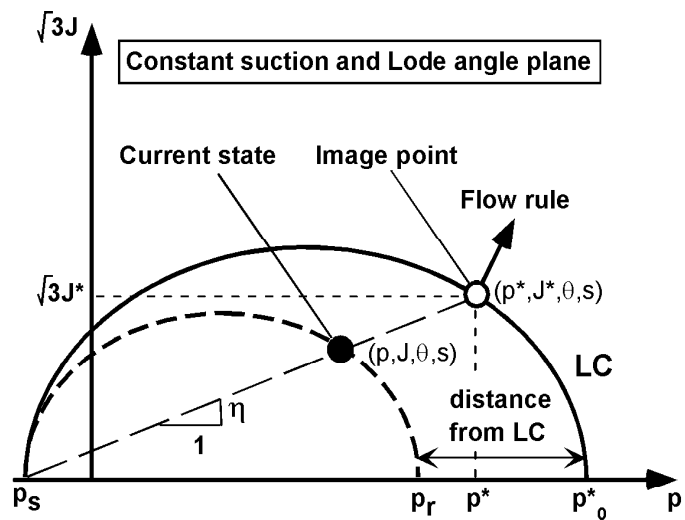
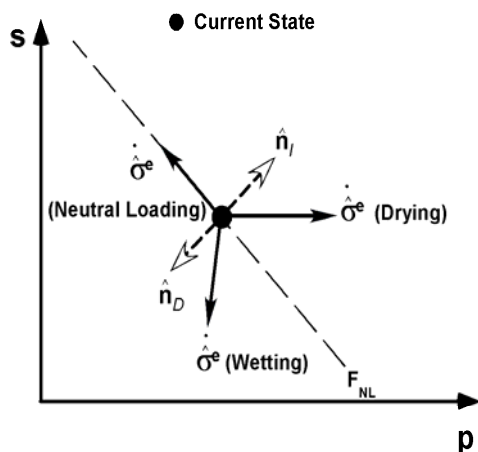
(Sánchez et al., 2005)



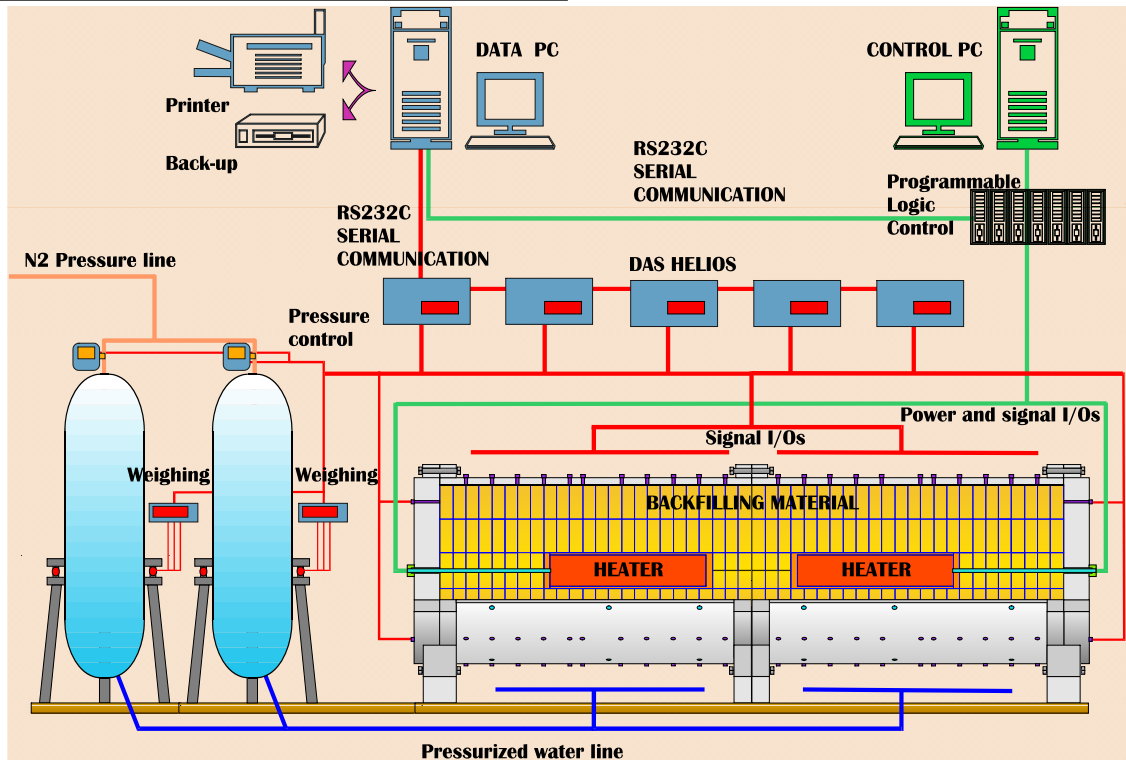
- Interaction between structural levels
- Loading/unloading direction
- Neutral line: $F_{NL} : p + s_i - \hat{p}_{NL} = 0$
- ◆ Drying criterion: $\dot{\sigma}^e : \hat{n}_I > 0$
- ◆ Wetting criterion: $\dot{\sigma}^e : \hat{n}_D > 0$
- ◆ Neutral loading: $\dot{\sigma}^e : \hat{n}_\beta = 0$

Generalised plasticity formulation

(Sánchez et al., 2005)



FEBEX mock up

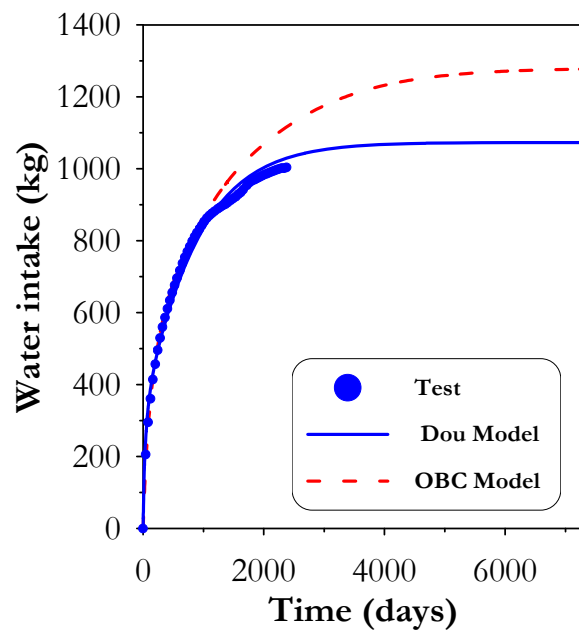
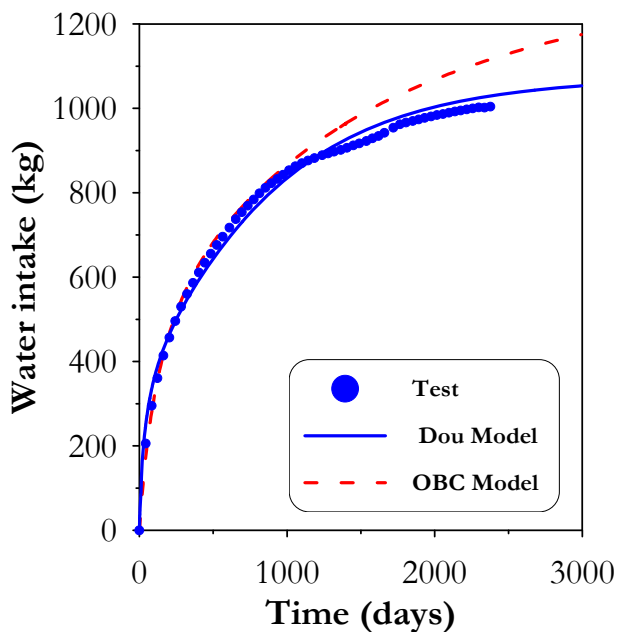


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▣ Mock up test: water inflow



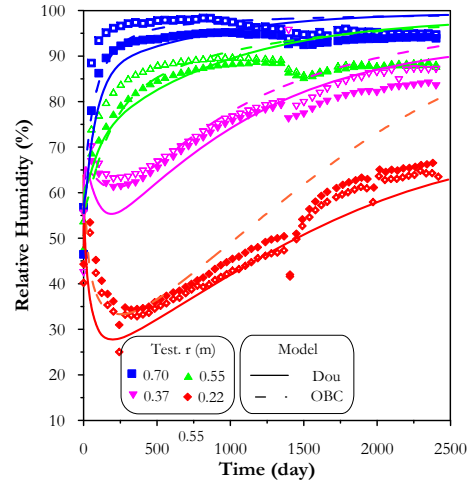
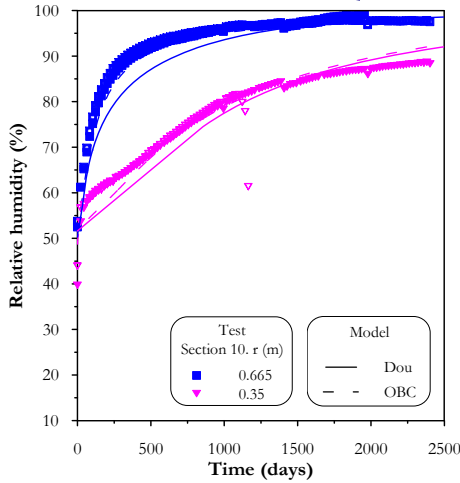
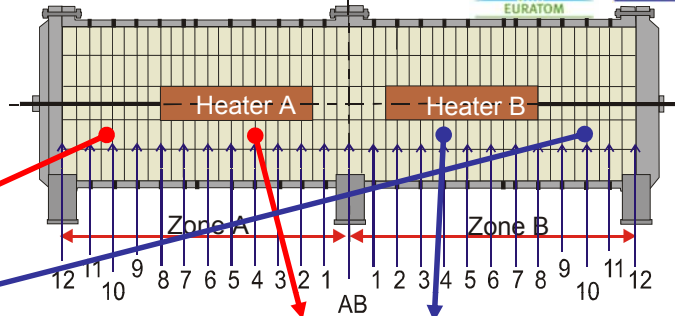
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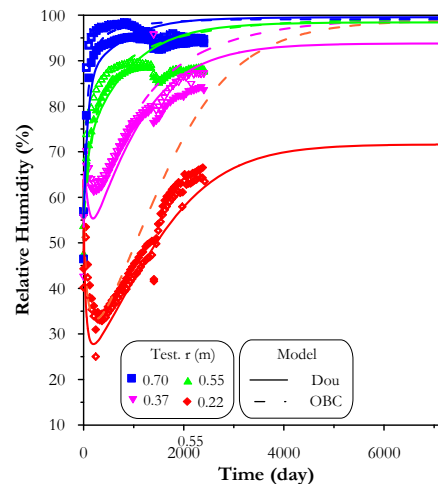
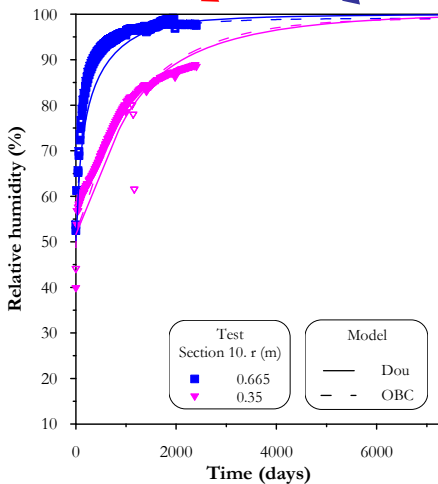
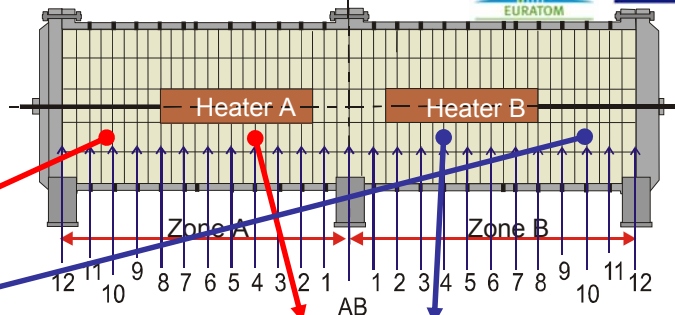
Double structure model

MOCK UP TEST
RELATIVE HUMIDITY



Double structure model

MOCK UP TEST
RELATIVE HUMIDITY



- ❑ Objectives
- ❑ THM modelling: HE-E test
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Threshold gradient

$$\mathbf{q}_l = -\mathbf{K}_l \mathbf{J}$$

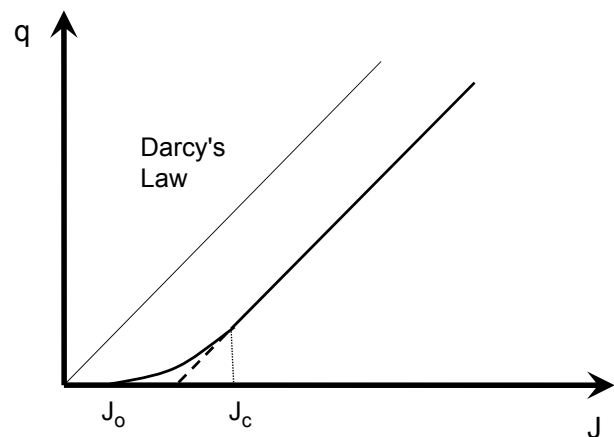
$$\mathbf{J} = \nabla \left(\frac{p}{\gamma_l} + z \right)$$

$$\mathbf{q}_l = -\mathbf{K}_l \left\langle \frac{J - J_0}{J} \right\rangle \mathbf{J}$$

J_c Critical Gradient = 1500

J_0 Threshold Gradient = 50

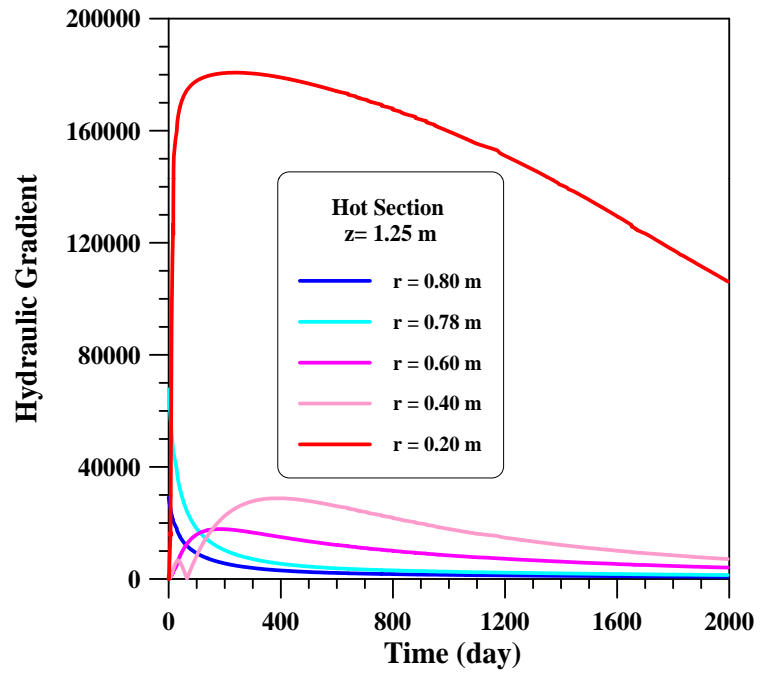
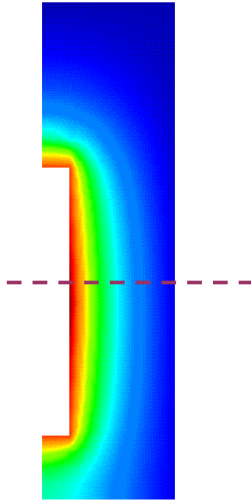
$$J = |\mathbf{J}|$$



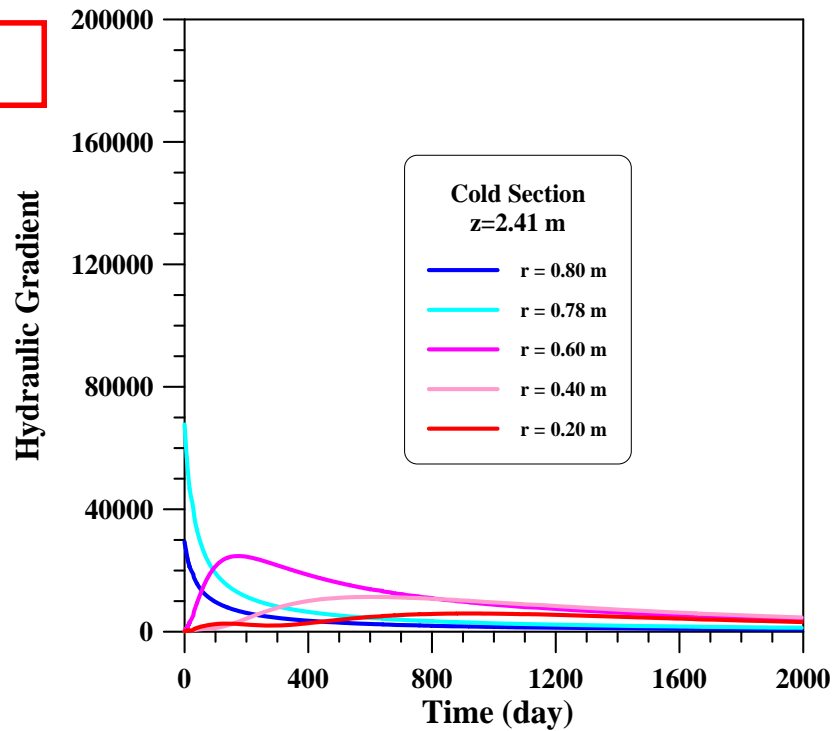
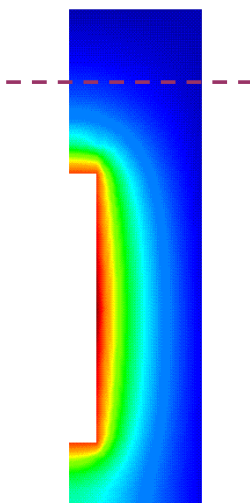
Generalized Darcy's Law

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu} \left\langle \frac{J - J_0}{J} \right\rangle^{n_t} (\nabla P - \rho \mathbf{g})$$

Radial Section



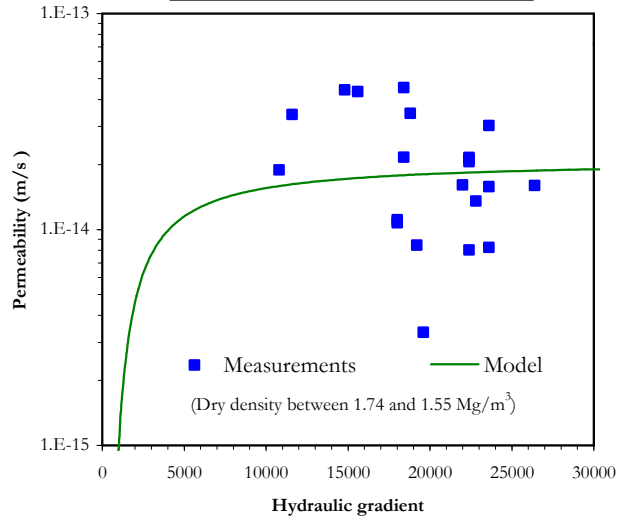
Radial Section



Threshold gradient

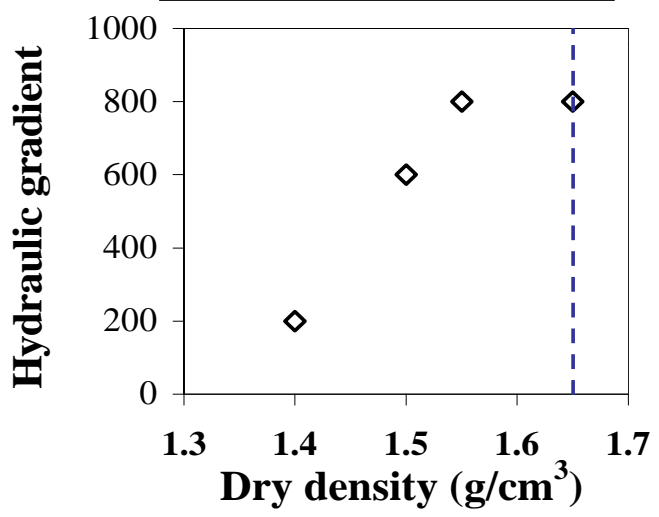
Experimental Data

Permeability determination



(Febex II report, 2004)

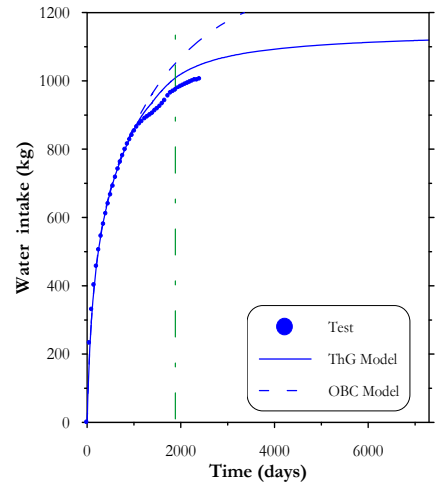
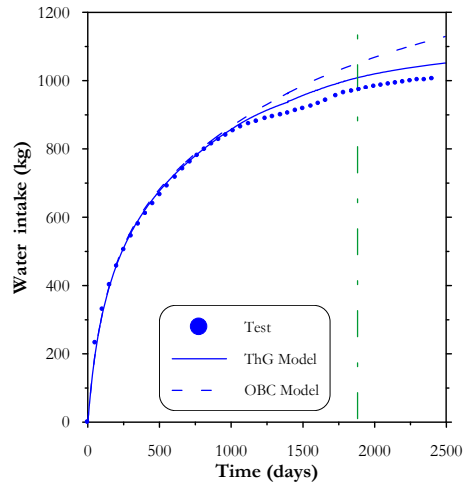
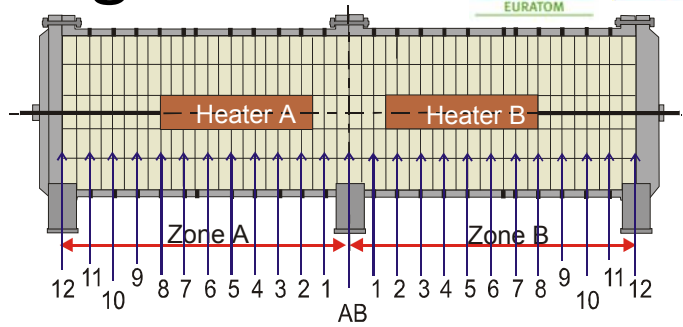
Minimum hydraulic gradient to get measurable flows



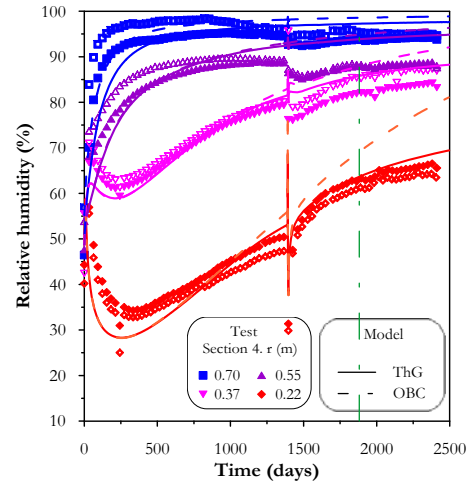
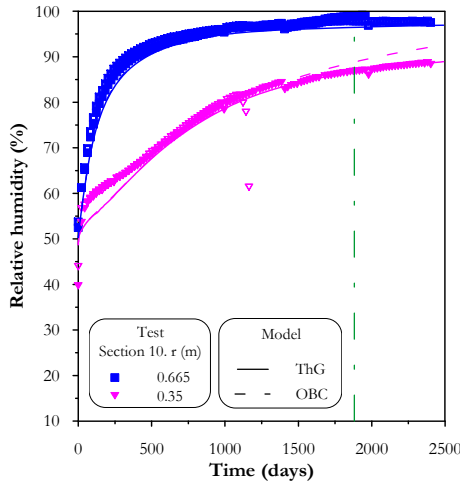
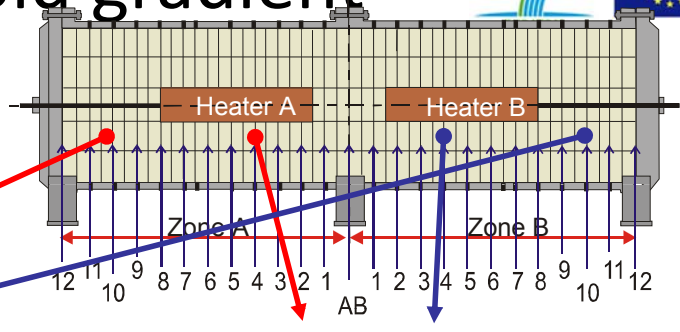
(Villar & Gómez, 2006)

Threshold gradient

MOCK UP TEST
WATER INFLOW



MOCK UP TEST
RELATIVE HUMIDITY



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□ Coupled processes and coupled phenomena

| | Gradients | | |
|---------|---|---------------------------|---------------------------------------|
| Flow | Hydraulic Head | Chemical Concentration | Temperature |
| Fluid | Darcy's Law (Hydraulic Conduction) | Chemical Osmosis | Thermo Osmosis |
| Solutes | Ultra Filtration | Fick's Law (Diffusion) | Soret Effect (Thermal Diffusion) |
| Heat | Thermo Filtration (Isothermal Heat Transfer) | Dufour Effect | Fourier's Law (Thermal Conduction) |

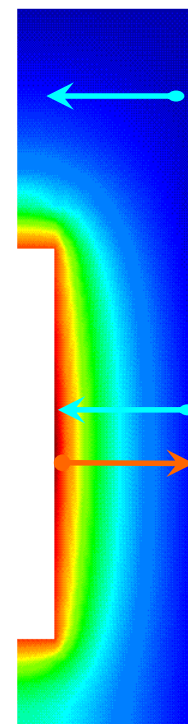
□ Thermo Osmosis

$$\mathbf{j}_l^w = \mathbf{i}_l^w + \theta_l^w \mathbf{q}_l + \theta_l^w S_l \dot{\mathbf{u}}$$

$$\mathbf{q}_l = -\mathbf{K}_{HH} (\nabla P_l - \rho_l \mathbf{g}) - \mathbf{K}_{HT} \nabla T$$

$$\mathbf{K}_{HT} = 2.73 \cdot 10^{-13} \text{ m}^2 / \text{K/s}$$

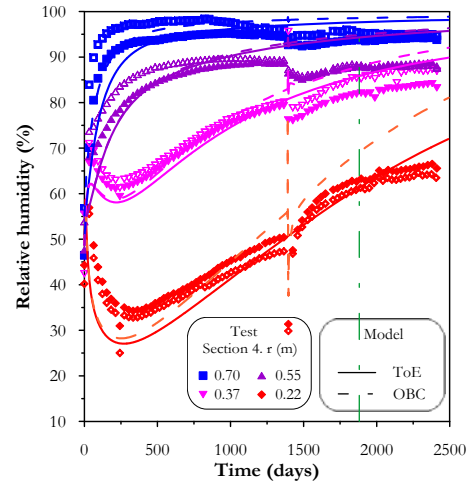
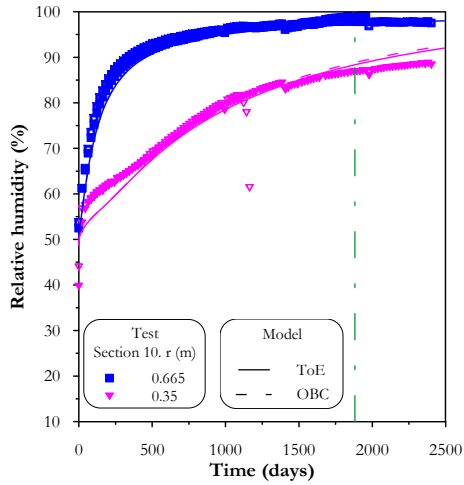
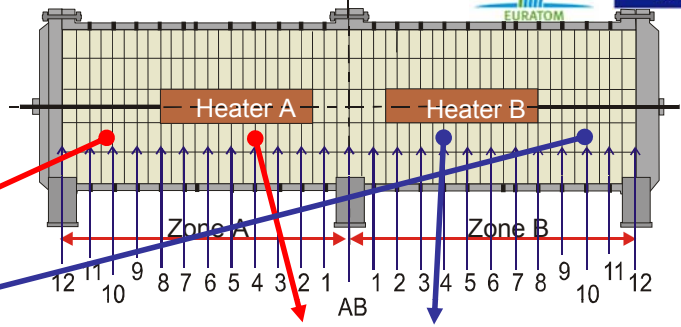
(Soler, 1999 ; Djeran, 1993)



Thermo-osmosis



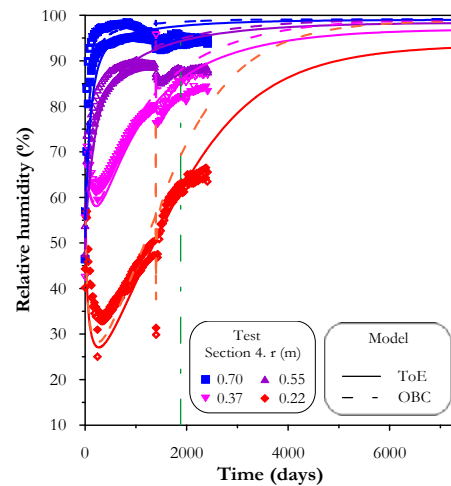
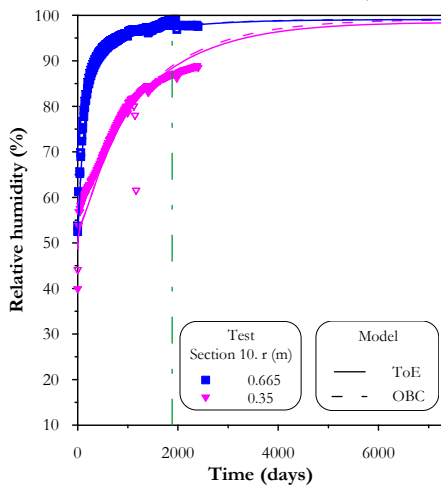
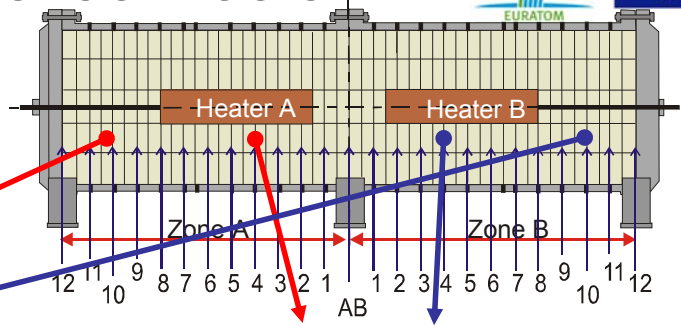
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RELATIVE HUMIDITY



Thermo-osmosis



MOCK UP TEST
RELATIVE HUMIDITY



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- ❑ Coupled processes and coupled phenomena

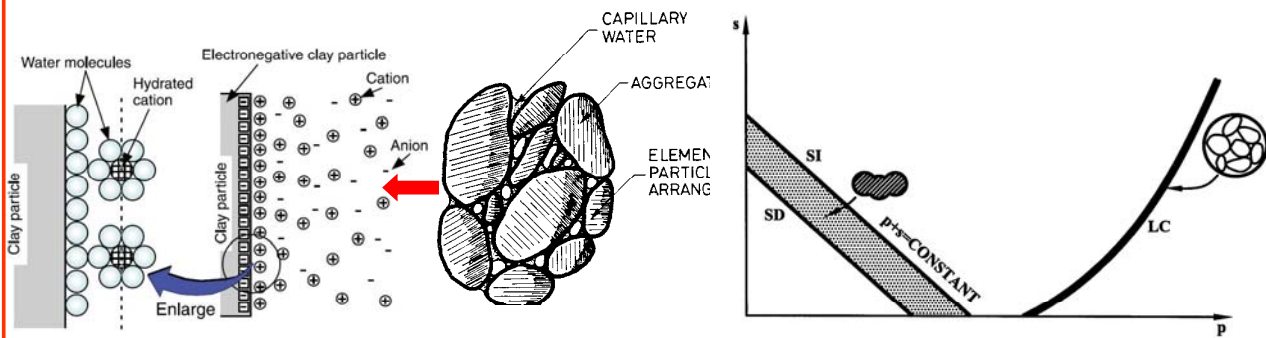
| | Gradients | | |
|----------------|---|-------------------------------|---------------------------------------|
| Flow | Hydraulic Head | Chemical Concentration | Temperature |
| Fluid | Darcy's Law (Hydraulic Conduction) | Chemical Osmosis | Thermo Osmosis |
| Solutes | Ultra Filtration | Fick's Law (Diffusion) | Soret Effect (Thermal Diffusion) |
| Heat | Thermo Filtration (Isothermal Heat Transfer) | Dufour Effect | Fourier's Law (Thermal Conduction) |

□ Double structure chemomechanical model

$$\Omega_m^e = -\frac{\beta_m}{\alpha_m} e^{-\alpha_m \hat{p}} \quad d\varepsilon_m^e = d\Omega_m^e = \beta_m e^{-\alpha_m \hat{p}} d\hat{p} - \frac{1}{\alpha_m} e^{-\alpha_m \hat{p}} d\beta_m$$

$$\beta_m = \sum_i \beta_m^i x_i \quad x_i = \frac{\text{exchangeable cation concentration}}{\text{CEC}} \quad \sum_i x_i = 1 \quad ; \quad 0 \leq x_i \leq 1$$

Chemical effects occur only in the microstructure



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□ Formulation for osmotic flow and hyperfiltration

○ Liquid flux

$$\mathbf{J}_l = \underbrace{-\rho_l k_l \nabla h_l}_{\text{water mass flow as a result of Darcy flow}} + \underbrace{\rho_l \sigma k_l \nabla s_o}_{\text{osmotic flow}} \quad s_o = RT \sum_{i=1}^N c_i \quad \text{Osmotic suction}$$

○ Solute flux

$$\mathbf{J}_i = \underbrace{c_i \rho_l \sigma k_l \nabla h_l}_{\text{hyperfiltration}} + \underbrace{\rho_l D_m^{eff} \nabla c_i}_{\text{molecular diffusion Fick Law}} - \underbrace{\rho_l \mathbf{D}'_l \nabla c_i}_{\text{mechanical dispersion}} + \underbrace{c_i (-\rho_l k_l \nabla h_l + \rho_l \sigma k_l \nabla s_o)}_{\text{advection}}$$

$$= -\rho_l \mathbf{D}'_l \nabla c_i - c_i \rho_l (1 - \sigma) k_l \nabla h_l + c_i \rho_l \sigma k_l \nabla s_o$$

○ Micro-macro chemical transfer

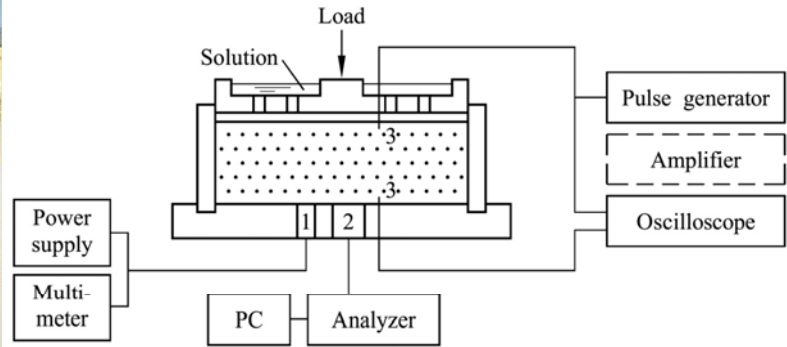
- There is a delay for transferring the chemical variable from the macrostructure to the microstructure

$$\frac{d\psi_m}{dt} = \beta \cdot [\psi_M - \psi_m] \quad \psi_M = s_o + \psi_c$$

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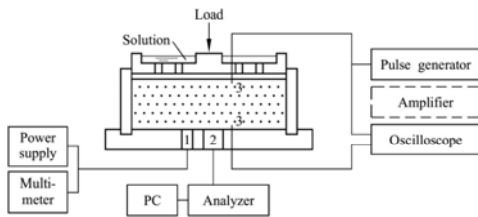
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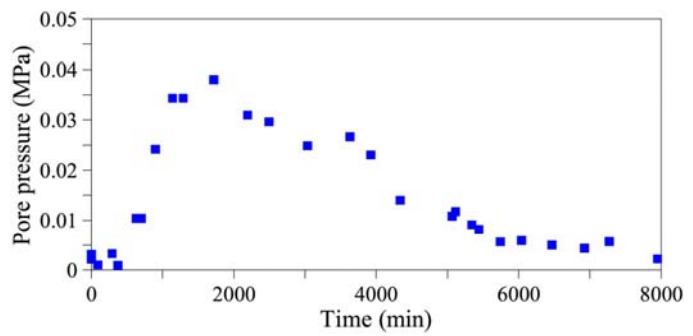
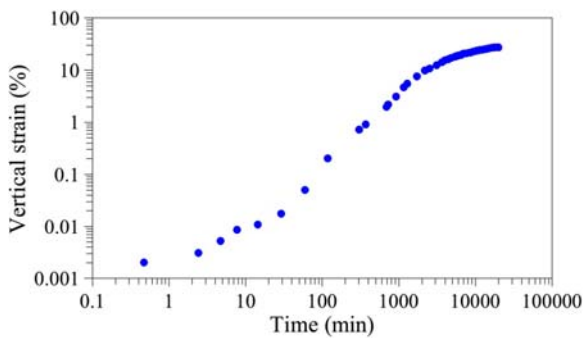


Na-bentonite sample
 1st stage: loading to 100 kPa
 2nd stage: KCl solution 4.0M

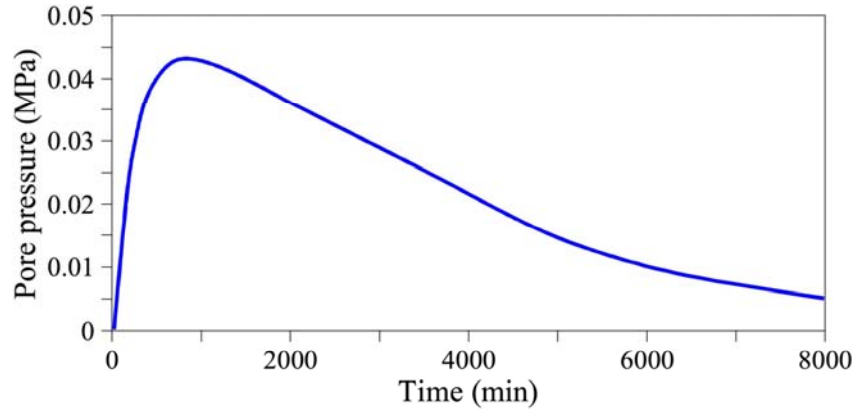
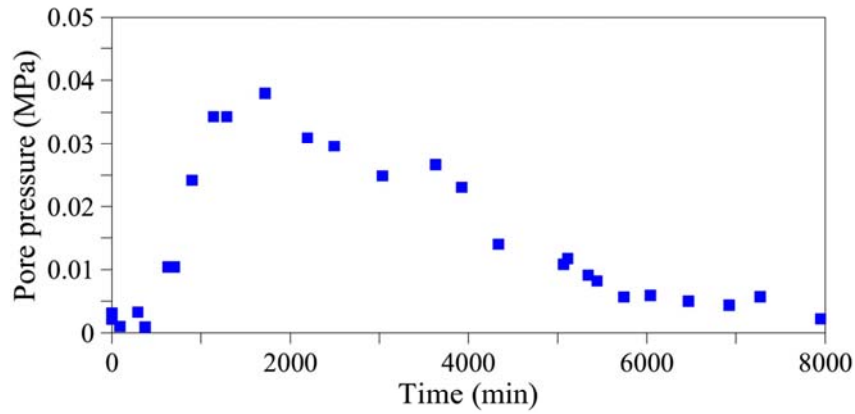
Modelling a chemomechanical oedometer test
 (Santamarina & Fam, 1995; Fam & Santamarina, 1996)



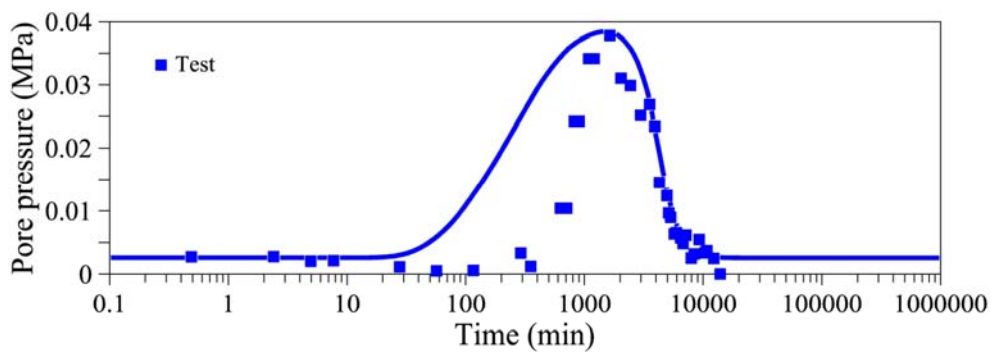
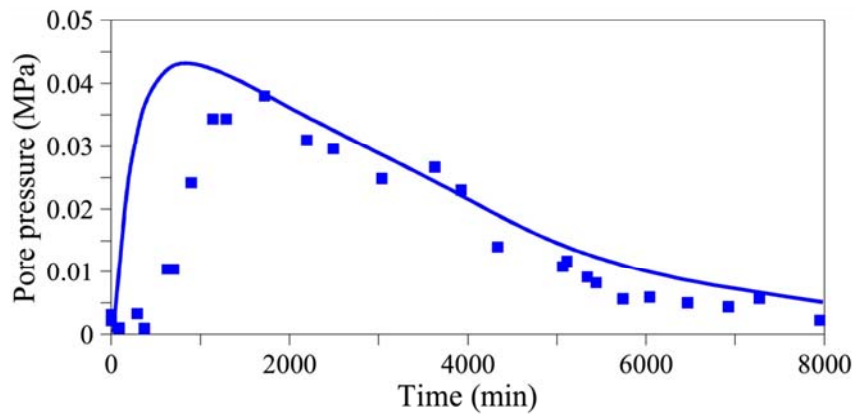
Bentonite sample
 1st stage: loading to 100 kPa
 2nd stage: KCl solution 4.0M



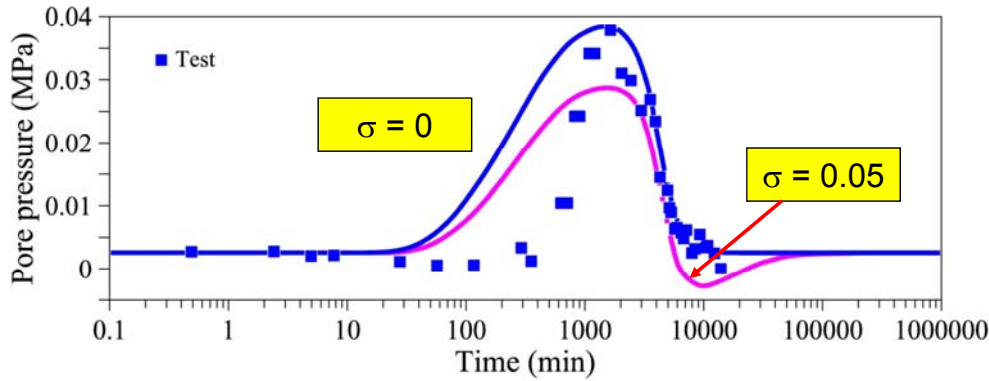
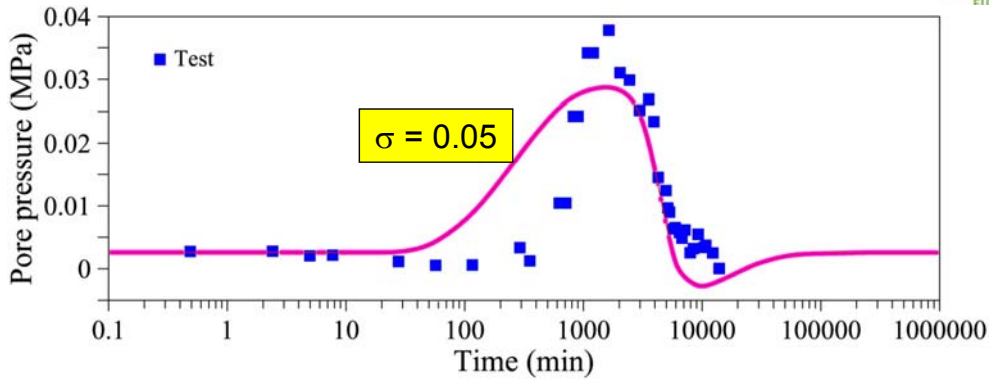
Osmotic flow



Osmotic flow

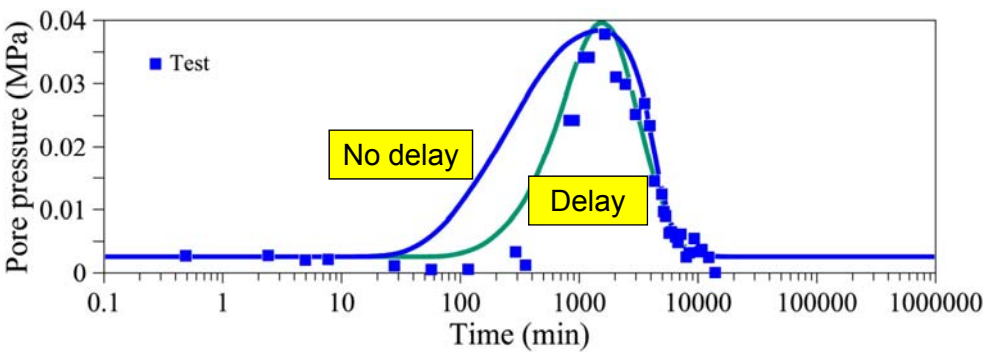
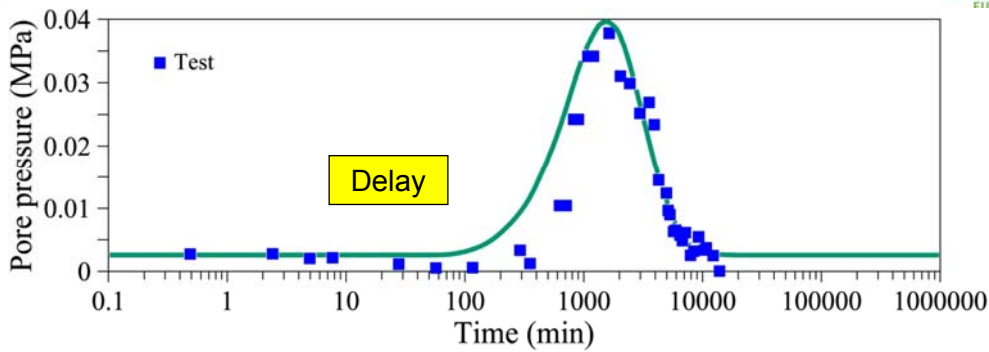


Osmotic flow

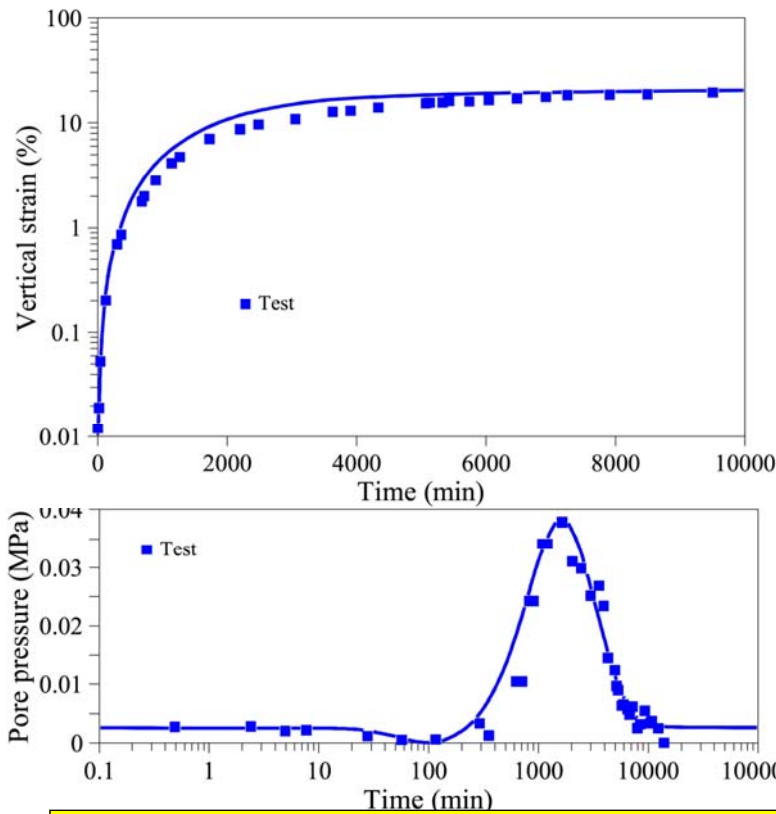


Osmotic flow ($\sigma = 0.05$ and $\sigma = 0$) No delay ($\beta = 0$)

Osmotic flow



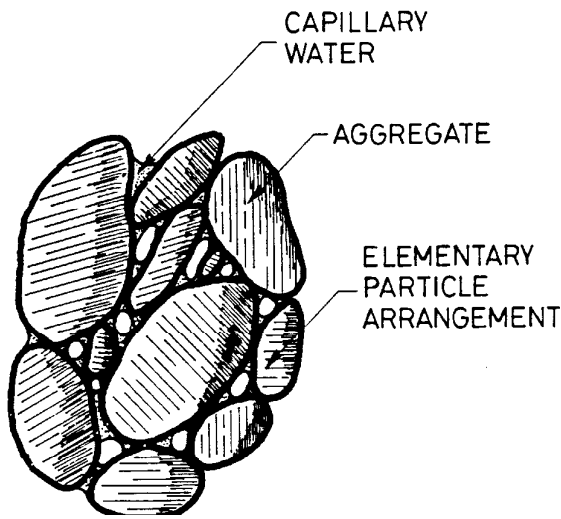
No osmotic flow ($\sigma = 0$) Delay ($\beta = 4.6 \times 10^{-7} \text{ s}^{-1}$)



Osmotic flow ($\sigma = 0.05\%$) Delay ($\beta = 4.6 \times 10^{-7} \text{ s}^{-1}$)

- ❑ Objectives
- ❑ THM modelling: HE-E test
- ❑ Incorporation of new features and some modelling results
 - Double structure model
 - Threshold gradient
 - Thermo-osmosis
 - Osmotic/flow – chemistry coupling
 - Water density

□ Constitutive model for a double structure material



(Sánchez et al., 2005)

□ Water density:

- Macrostructure water: constant density = 1.0 Mg/m³
- Microstructure water: density varying with suction

□ A general THM formulation

MASS BALANCE OF SOLID

$$\frac{D\phi}{Dt} = \frac{D\phi_M}{Dt} + \frac{D\phi_m}{Dt} = \frac{(1-\phi) D\rho_s}{\rho_s Dt} + (1-\phi_M - \phi_m)(\dot{\epsilon}_{vM} + \dot{\epsilon}_{vm})$$

MASS BALANCE OF WATER

$$\frac{\partial}{\partial t} (\rho_w S_{wj} \phi_j) + \nabla \cdot (\mathbf{j}_{wj}) \pm \Gamma^w = f_j^w ; j = M, m$$

MOMENTUM BALANCE FOR THE MEDIUM

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}$$

$$\frac{\partial}{\partial t} (E_s \rho_s (1-\phi) + E_l \rho_l S_l \phi + E_g \rho_g S_g \phi) + \nabla \cdot (\mathbf{i}_c + \mathbf{j}_{Es} + \mathbf{j}_{El} + \mathbf{j}_{Eg}) = f^Q$$

Mass balance of microstructure and macrostructure water density

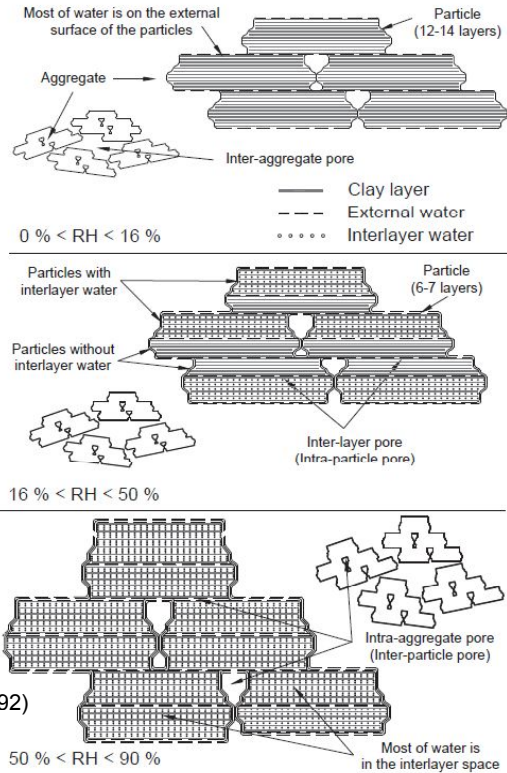
Microstructure

$$\frac{\partial}{\partial t} (\rho_{wm}(\psi_m) S_{wm} \phi_m) + \nabla \cdot (\mathbf{j}_{wm}) + \Gamma^w = 0$$

Macrostructure

$$\frac{\partial}{\partial t} (\rho_{wM} S_{wM} \phi_M) + \nabla \cdot (\mathbf{j}_{wM}) - \Gamma^w = f_j^w$$

$$\Gamma^w = \gamma \cdot [\psi_M - \psi_m]$$



Microstructural water density

$$\frac{\partial}{\partial t} (\rho_{wm}(\psi_m) S_{wm} \phi_m) + \nabla \cdot (\mathbf{j}_{wm}) + \Gamma^w = 0$$

$$\rho_w^j = \frac{w_j}{S_{int,j} \Delta_j}$$

Theoretical water density in the interlayer space

$$w_j = \frac{j S_{int,j} M_w}{2 \sigma_j N_A}$$

Theoretical interlayer water content

$$\rho_w^i = \frac{\sum_{j=1}^n p_j w_j}{\sum_{j=1}^n p_j \frac{w_j}{\rho_w^j}}$$

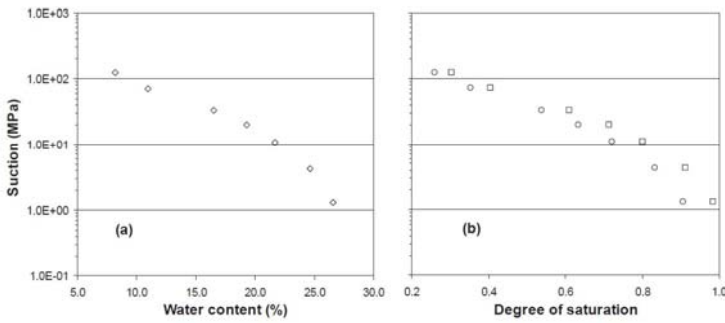
Interlayer water density

(Jacinto, 2010)

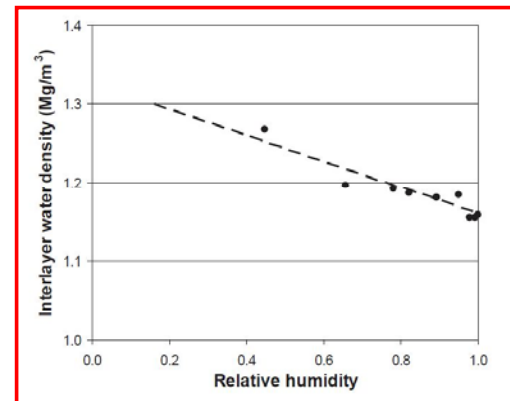
Microstructural water density: MX-80

| Water layers j | ρ_w^j (Mg/m ³) |
|------------------|---------------------------------|
| 1 | 1.32 |
| 2 | 1.17 |
| 3 | 1.16 |
| 4 | 1.14 |

| Suction (MPa) | RH | Layers | | | | |
|---------------|------|--------|------|------|------|------|
| | | 0 | 1 | 2 | 3 | 4 |
| 0.01 | 1.00 | 0.0 | 0.0 | 0.32 | 0.32 | 0.20 |
| 0.03 | 1.00 | 0.0 | 0.0 | 0.32 | 0.32 | 0.20 |
| 0.10 | 1.00 | 0.0 | 0.0 | 0.20 | 0.60 | 0.20 |
| 1.0 | 0.99 | 0.0 | 0.0 | 0.33 | 0.33 | 0.33 |
| 2.8 | 0.98 | 0.0 | 0.0 | 0.33 | 0.33 | 0.33 |
| 6.9 | 0.95 | 0.0 | 0.22 | 0.50 | 0.28 | 0.0 |
| 15.0 | 0.89 | 0.0 | 0.15 | 0.70 | 0.15 | 0.0 |
| 26.0 | 0.82 | 0.0 | 0.23 | 0.60 | 0.17 | 0.0 |
| 33.0 | 0.78 | 0.0 | 0.30 | 0.50 | 0.20 | 0.0 |
| 56.0 | 0.66 | 0.10 | 0.30 | 0.50 | 0.10 | 0.0 |
| 107.0 | 0.45 | 0.18 | 0.64 | 0.18 | 0.0 | 0.0 |



(Jacinto, 2010)



Summary

- ❑ Some predictive modelling results of the HE-E (WP3.2) have been presented.
- ❑ These modelling results (WP3.2) and those from the EB experiment (WP3.1) and from the FEBEX mock up (WP3.3) will be improved by incorporating some new features
 - Double structure model
 - Threshold gradient
 - Thermo-osmosis
 - Osmotic/flow – chemistry coupling
 - Water density
- ❑ The parameters of these new features will be calibrated on an independent (considering one process at a time) (WP3.3) basis from existing and new (WP2) laboratory data. The mutual influence of each of the new processes will be assessed.
- ❑ Long term predictions will be carried out using the updated model (WP3.5)

“The research leading to these results has received funding from the European Atomic Energy Community's Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 249681”

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