

Numerical analysis of coupled hydro-mechanical and thermo-hydro-mechanical behaviour in buffer materials at a geological repository for nuclear waste: Simulation of EB experiment at Mont Terri URL and FEBEX at Grimsel test site using Barcelona basic model

Lee,C. , Lee,J. , Kim,GY.

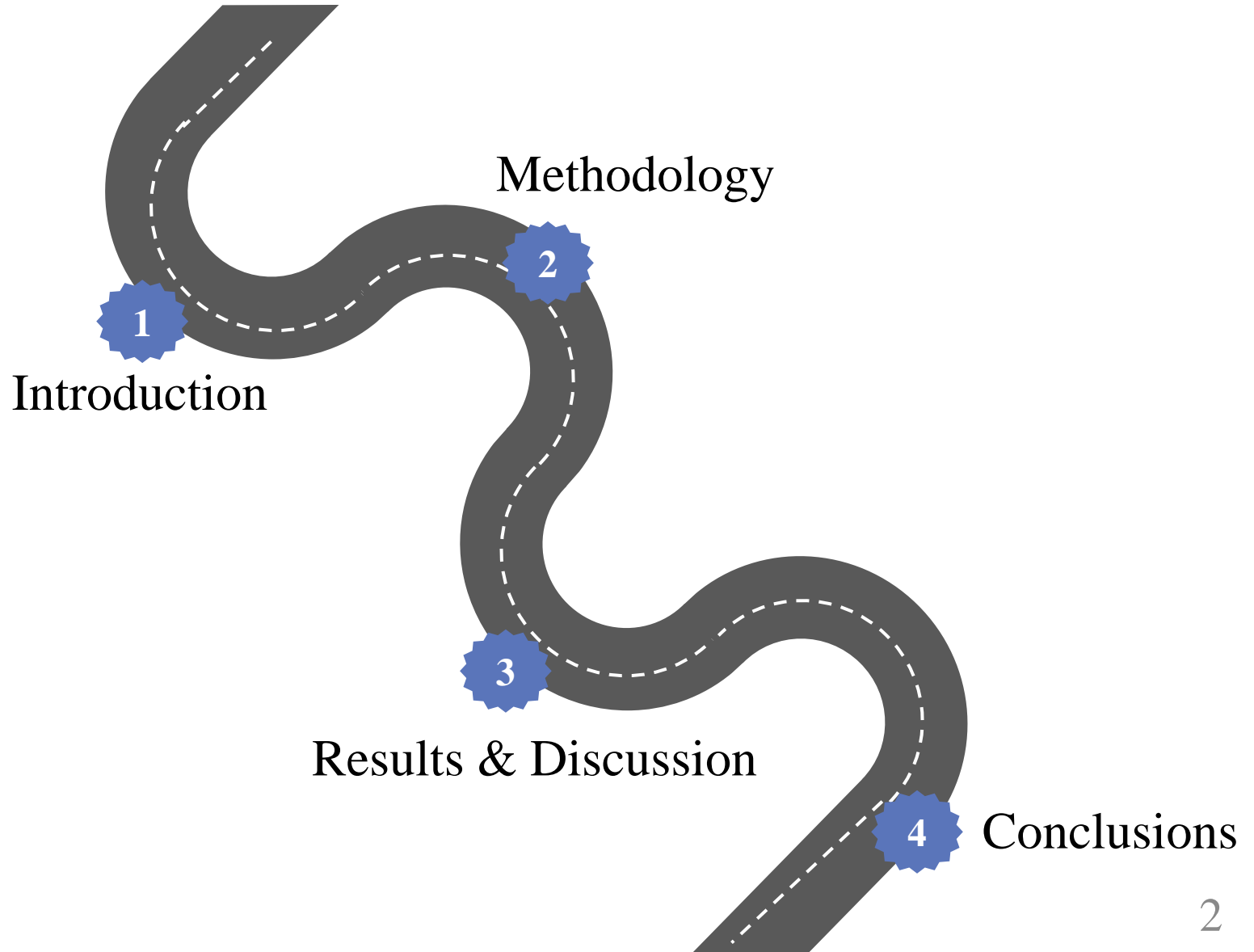
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Date : 2022/12/23

# Outline



# Introduction

## Deep Geological Disposal

- Spent nuclear fuel has **high level of radioactivity** and a long **half-life**. This type of radioactive wastes is called **high-level radioactive waste(HLW)**.
- Seeking appropriate environmental disposal **to isolate HLW from the biosphere**.
- The concept of **multiple barriers**, the spent nuclear fuel is buried in the geology below 300~1000 meters, and then the canister and buffer materials are used to cover and place.

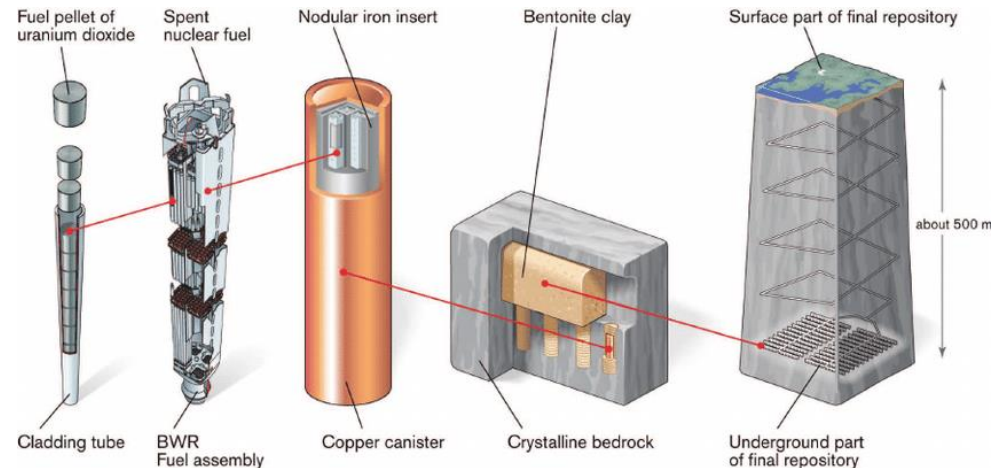
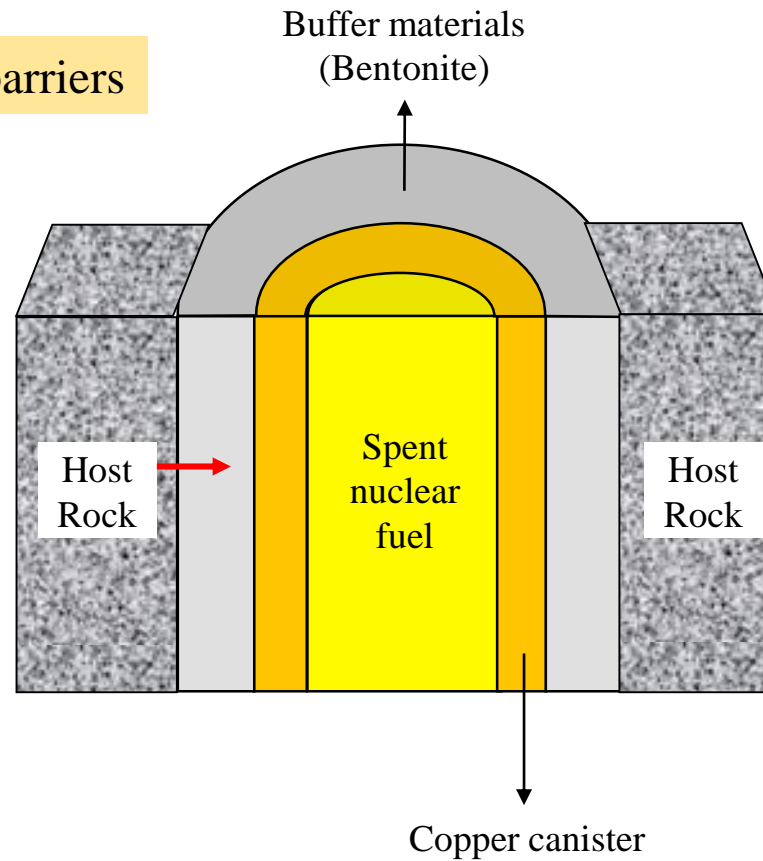


Fig. 1. Design Concept for the Deep Geological Disposal (Swedish KBS-3 method)

# Coupled THMC process

( Thermo-hydro-mechanical-chemical )

Multiple barriers



# Coupled THMC process ( Thermo-hydro-mechanical-chemical )

**T** The radioactive wastes emits heat by radiation decay  
→ cause temperature rise

**M** The rise temperature produces water evaporation and condenses in cooler areas, so the buffer material is shrinking and swelling.

**H** Buffer materials is unsaturated, under suction, groundwater flows from the host rock to the buffer.

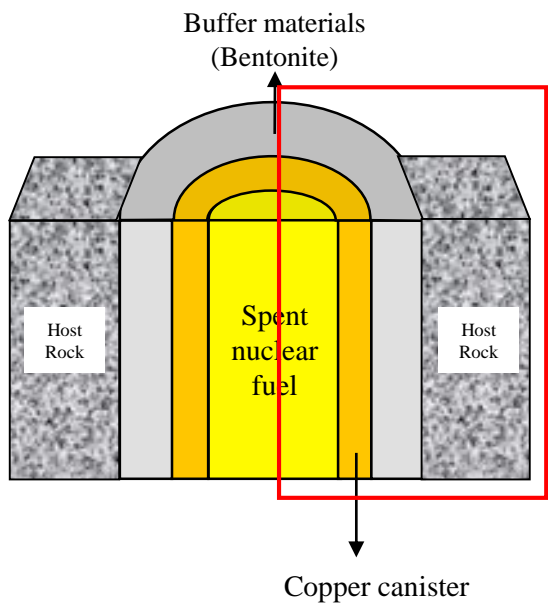


Fig. 2-1. Schematic cross-section (reference from Rebecca Lunn)

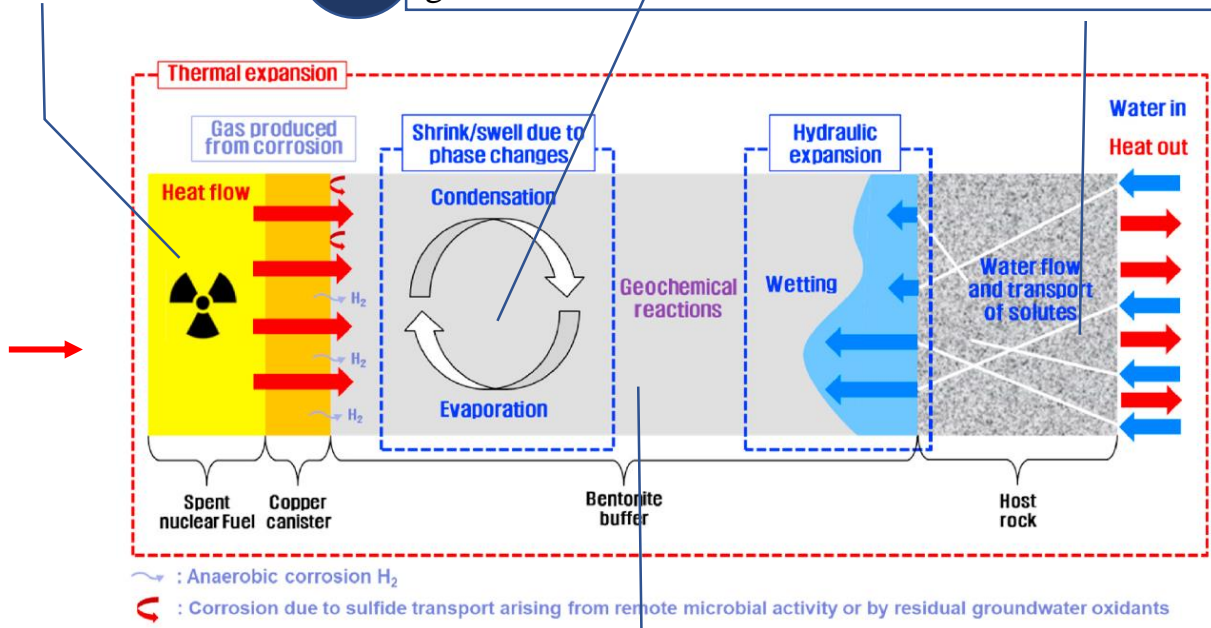


Fig. 2-2. Schematic of the coupled THMC processes in the HLW disposal system.

**C** Colloids are carried into the groundwater and cause progressive erosion of the buffer material.

## Coupled THMC process

( Thermo-hydro-mechanical-chemical )

- **The coupled THMC processes play important roles** in the design, construction, and operation of a repository in deep geological formations.
- However, it is difficult to combine the complex coupled THMC processes into efficient models and develop numerical techniques to simulate them.

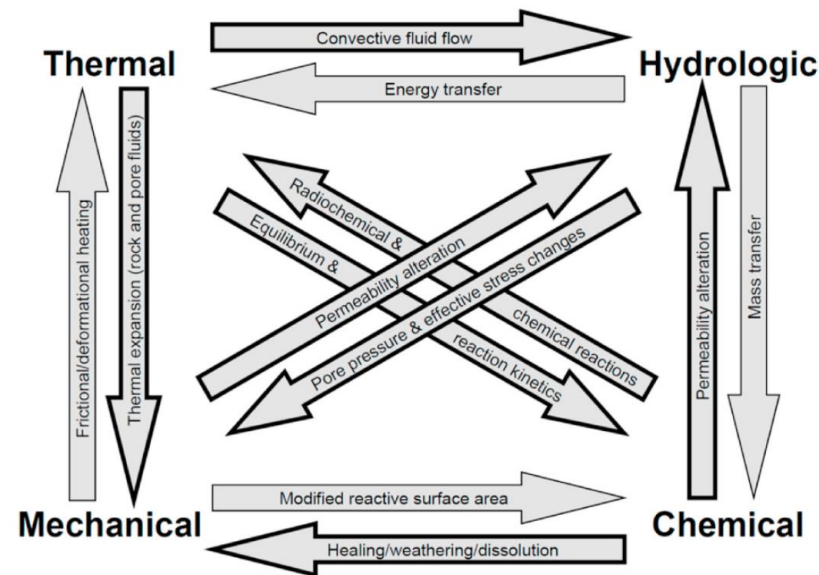


Fig.3. Coupled THMC processes in the repository for HLW.

## Objective

- To solve these problems, an international cooperative project called DECOVALEX is to study HM and THM interactions. **Special attention was paid to the evolution of barrier heterogeneity under transient conditions and the final state of the barrier.**

The logo for DECOVALEX 2019. The word "DECOVALEX" is in a bold, black, sans-serif font. Below it, the year "2019" is written in a large, blue, sans-serif font. The "0" in "2019" is stylized with a white circular center and blue lines radiating from it, resembling a globe or a cross-section of a material. The "1" and "9" also have blue lines radiating from them, giving the entire logo a dynamic, textured appearance.



## Two in-situ experiments

### The EB (Engineered barrier) test

- Site ▶ Mont Terri URL
- Rock mass ▶ Opalinus clay
- Barrier type ▶ Granular bentonite (GBM) and bentonite blocks.
- Hydration ▶ **Artificial hydration**
- Total duration ▶ 10.7 years
- Observe ▶ coupled HM behavior

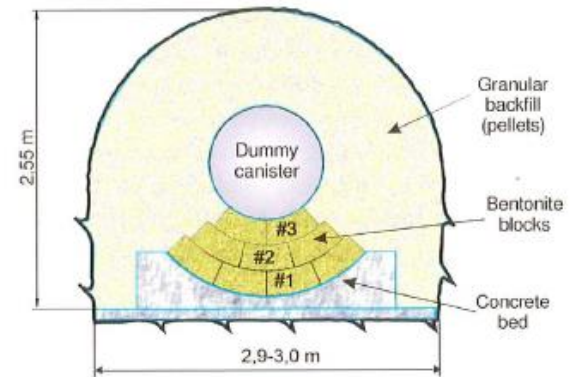


Fig.3-1. EB experimental layout

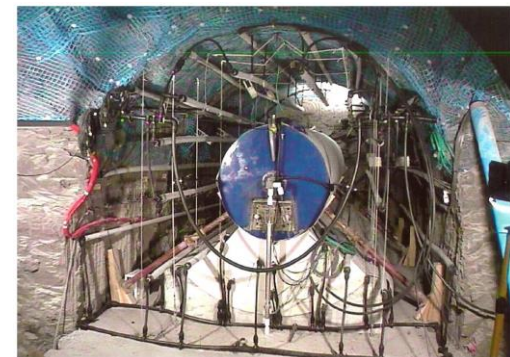


Fig.3-2. Canister sitting on a bed of compacted bentonite blocks.

## Two in-situ experiments

## The FEBEX (Full-scale Engineered Barrier EXperiment) test

- Site ▶ Grimsel Test Site
- Rock mass ▶ crystalline rock (Granite)
- Heater ▶ **Non-isothermal test**
- Barrier type ▶ Bentonite blocks
- Hydration ▶ **Natural hydration**
- Total duration ▶ 18.4 years
- Observe ▶ coupled THM behavior

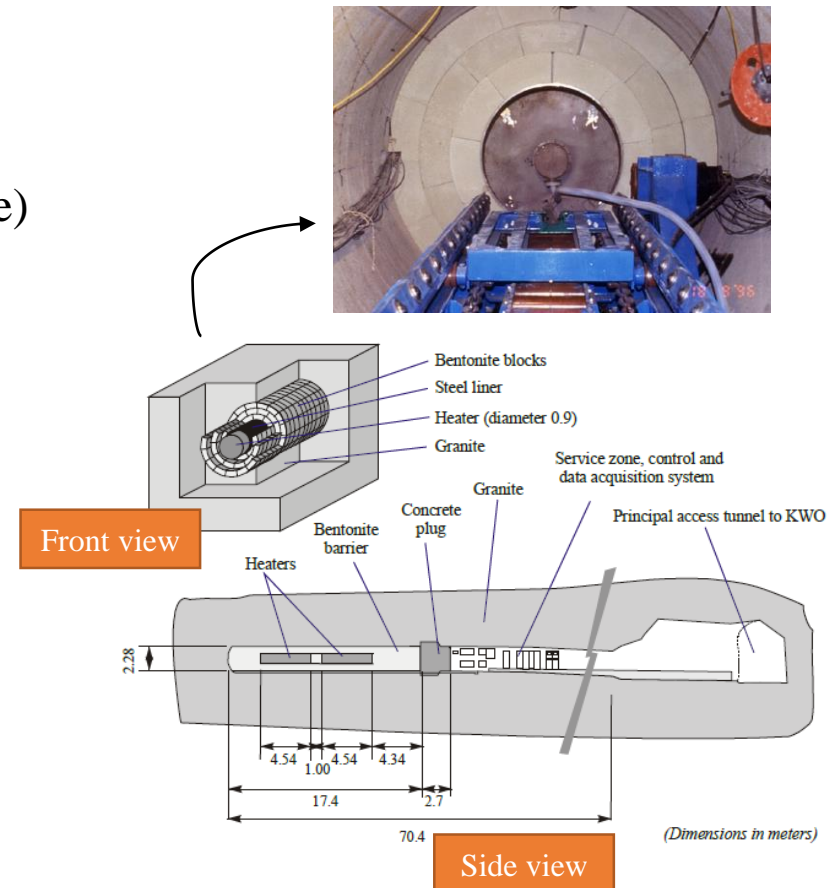


Fig.3-2. FEBEB experimental layout

# Methodology

# Numerical simulator

- Using a **TOUGH2-MP/FLAC3D** simulator to represent the coupled behaviour in bentonite buffer materials at the two long-term in situ experiments.
- **TOUGH2-MP** (Transport Of Unsaturated Groundwater and Heat) is a numerical simulation program for nonisothermal flows of multicomponent, multiphase fluids in porous and fractured media.
- **FLAC3D** (Fast Lagrangian Analysis of Continua in 3D) is to solve complex geotechnical problems for three-dimensional analyses of soil, rock, concrete, structural ground support, and groundwater flow.

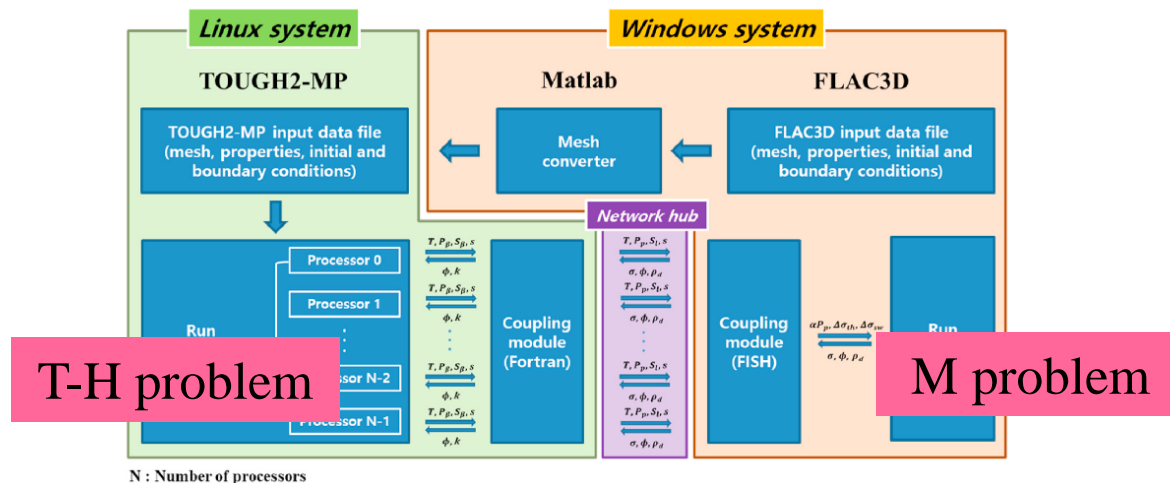


Fig. 4. TOUGH2-MP/FLAC3D coupling algorithm

## Mathematical formulations

- Balance equations

(a.) The total mass balance equation of the fluid

$$\frac{d}{dt} \varphi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^k + \nabla \cdot \left( \sum_{\beta} X_{\beta}^k \rho_{\beta} u_{\beta} - \sum_{\beta} \bar{D}_{\beta}^k \rho_{\beta} \nabla X_{\beta}^k \right) = Q_{\beta}$$

$k$  is component (air or water)

$\beta$  is phase (gas or liquid)

$\varphi$  is porosity

$S_{\beta}$  is the saturation of phase  $\beta$

$\rho_{\beta}$  is the density of phase  $\beta$

$X_{\beta}^k$  is the mass fraction of component  $k$

$u_{\beta}$  is the Darcy velocity in phase  $\beta$

$\bar{D}_{\beta}^k$  is the hydrodynamic dispersion tensor of  $k$  in phase  $\beta$

$Q_{\beta}$  is the fluid source or the sink term in phase  $\beta$

# Mathematical formulations

- Balance equations

## (b.) The heat transfer

$$\frac{d}{dt} \left( (1 - \varphi) \rho_R C_R T + \varphi \sum_{\beta} S_{\beta} \rho_{\beta} u_{\beta} \right) + \nabla \cdot \left( -\lambda \nabla T + \sum_{\beta} h_{\beta} F_{\beta} \right) = Q$$

$\varphi$  is porosity

$\rho_R$  is the grain density of the matrix

$C_R$  is the specific heat of the matrix

$S_{\beta}$  is the saturation of phase  $\beta$

$\rho_{\beta}$  is the density of phase  $\beta$

$u_{\beta}$  is the specific internal energy in phase  $\beta$

$\lambda$  is the effective thermal conductivity

$h_{\beta}$  is the specific enthalpy in phase  $\beta$

$F_{\beta}$  is the phase flux

$Q$  is the energy source or sink term

## (c.) The momentum balance equation

$$\nabla \cdot \sigma + b = 0$$

$\sigma$  is a stress tensor

$b$  is a vector of body forces

# Numerical modelling

## The EB test

- The domain was 20 m wide, 40 m high, and 0.1 m thick with a central plane of symmetry. The mesh contains 16,534 elements and 17,050 grid points.

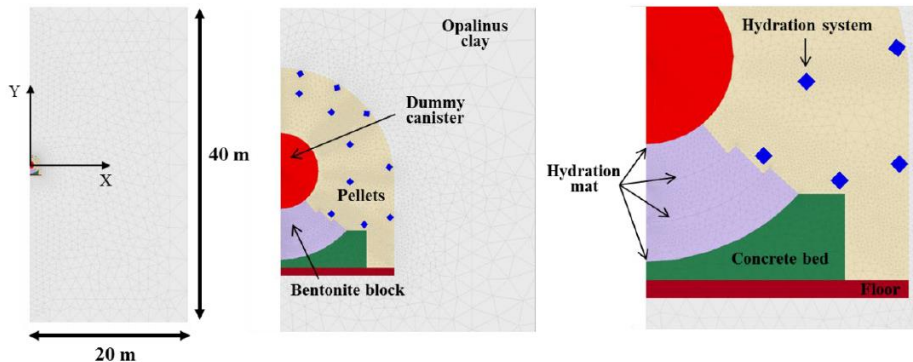


Fig.5-1. Plane strain domain for EB test

Table 1. Stages of the EB test

Stage No.	Description	Start time (day)	Duration (days)
1	Excavation and tunnel ventilation	-160	160
2	Installation	0	5
3	1 <sup>st</sup> artificial hydration	5	2
4	Natural hydration only	7	125
5	2 <sup>nd</sup> artificial hydration	132	324
6	3 <sup>rd</sup> artificial hydration	456	1003
7	4 <sup>th</sup> artificial hydration	1459	416
8	Natural hydration only	1872	2036

# Numerical modelling

## The FEBEX test

- The domain was 120 m length (X) and 50 m radius (Y) with 6966 elements and 14,277 grid points.

Table 2. Stages of the FEBEX test

Stage No.	Description	Start time (day)
1	Tunnel excavation and ventilation	-385
2	Installation of the experiment	-135
3	1200 W applied by each heater	0
4	2000 W applied by each heater	20
5	Controlled temperature of the heaters: 100 °C	53
6	Heater #1 switched off and first dismantling	1827
7	Construction of the shotcrete plug	1966
8	Controlled temperature of heater #2: 100 °C	1974
9	Heater #2 switched off	6630
10	Final dismantling	6758

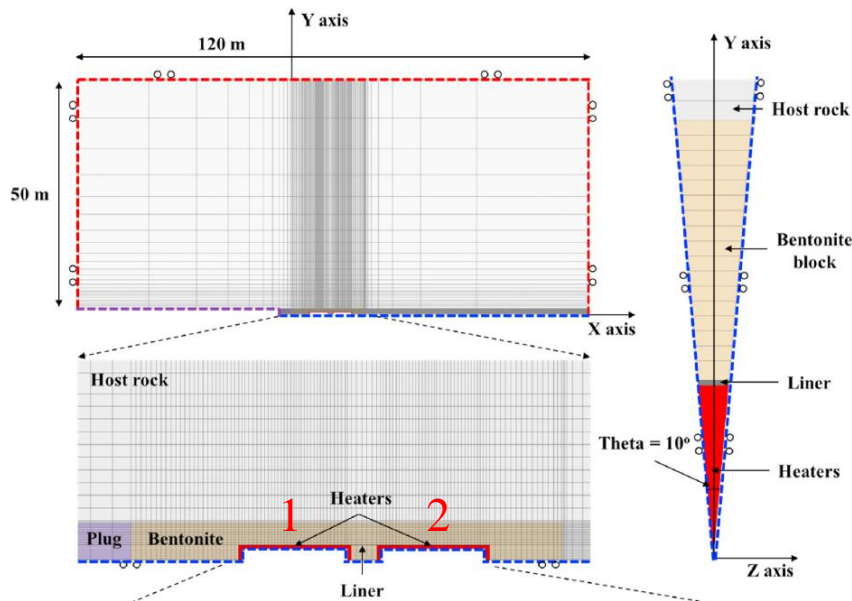


Fig.5-2. Plane strain domain for FEBEX test



# Results & Discussion

## EB test

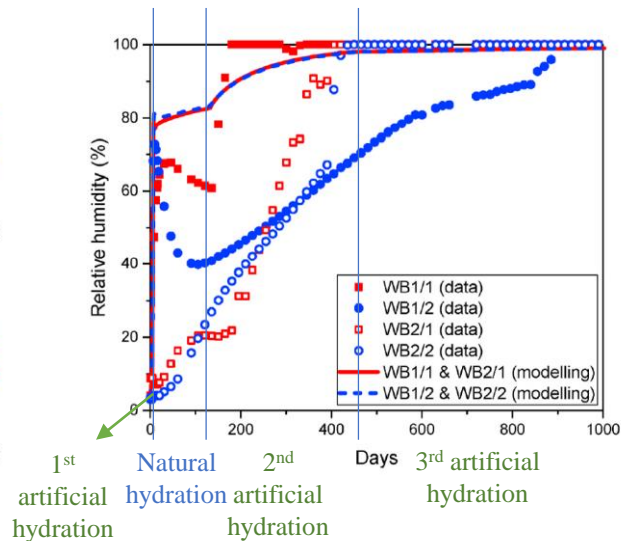
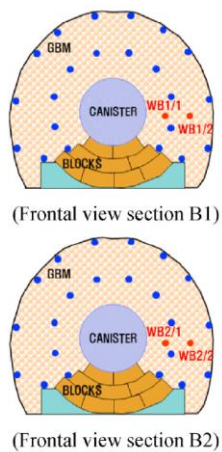
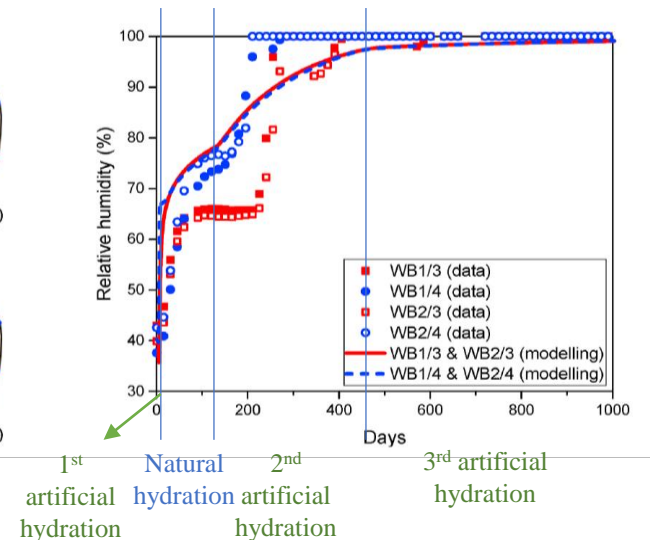
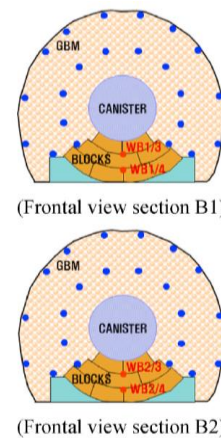
relative humidity sensor  
on GBMrelative humidity sensor  
on bentonite blocks

Fig.6-1. Evolution of relative humidity at Sections B1 and B2



The modelling result of bentonite blocks is more satisfy with in-situ data than GBM.

- On GBM found that **leakages** through the Opalinus Clay formation and the concrete plug.
- The amount of water losses could not be quantified in the in-situ experiment.

## EB test

## Dry density

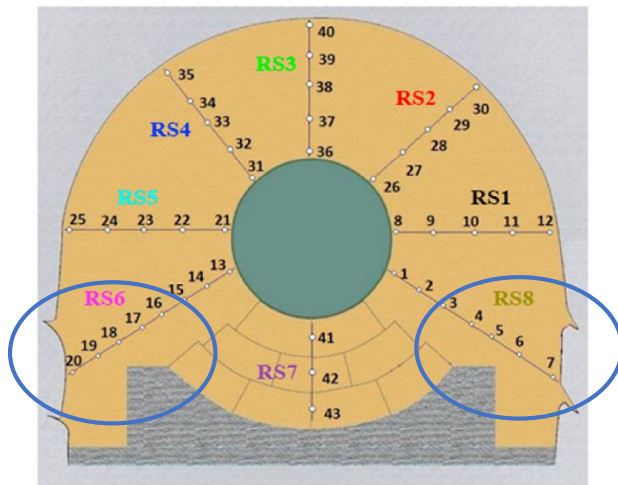


Fig. Divided into eight radial segments at Sections B2

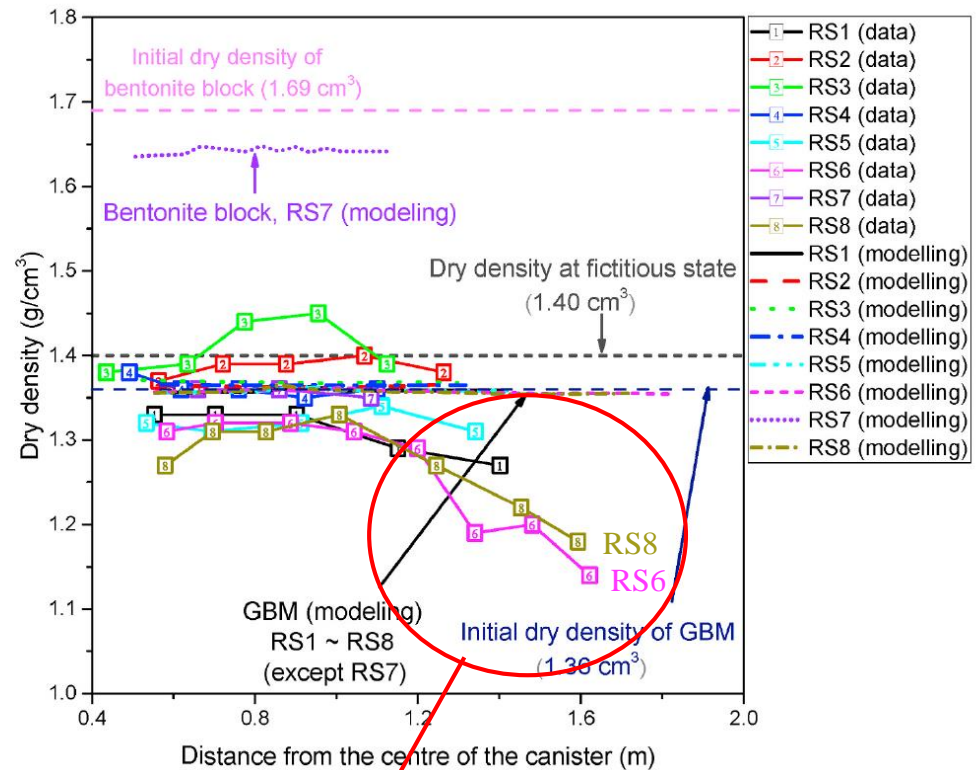


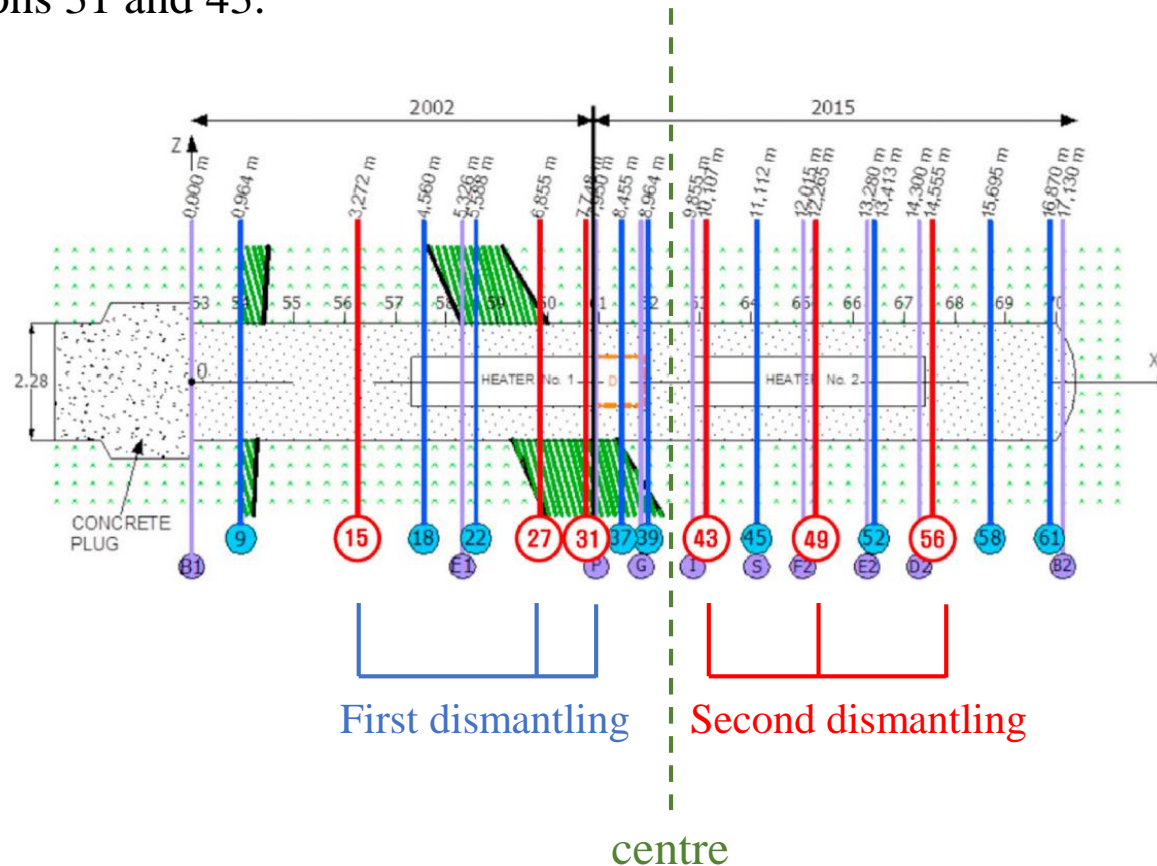
Fig. Distribution of dry density



There are damage zone with high permeability at the corner due to the stress concentration, so most of water may have leaked through the corners.

## FEBEX test

- Base on the distance from the centre of the two heaters, it investigate the difference between the observations after the first and second dismantling.
- The six sections were divided into three groups, sections 15 and 56, sections 27 and 49, and sections 31 and 43.



## FEBEX test

## Heater power

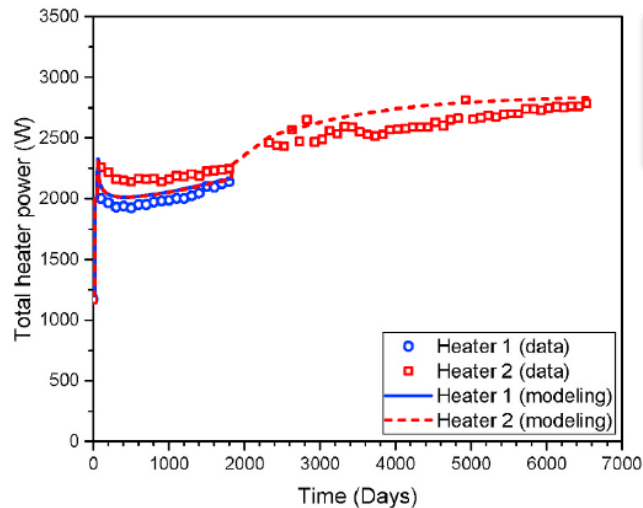


Fig.8. Total heater power of heaters #1 and #2



approximately 10% of the difference between the power values could not be reproduced in the numerical simulations

- 1** Because all bentonite blocks were assumed to have been simultaneously installed in the numerical simulations.
- 2** The rock mass was assumed to be a homogeneous medium without considering the presence of lamprophyre with low thermal conductivity.

# FEBEX test

## Water content

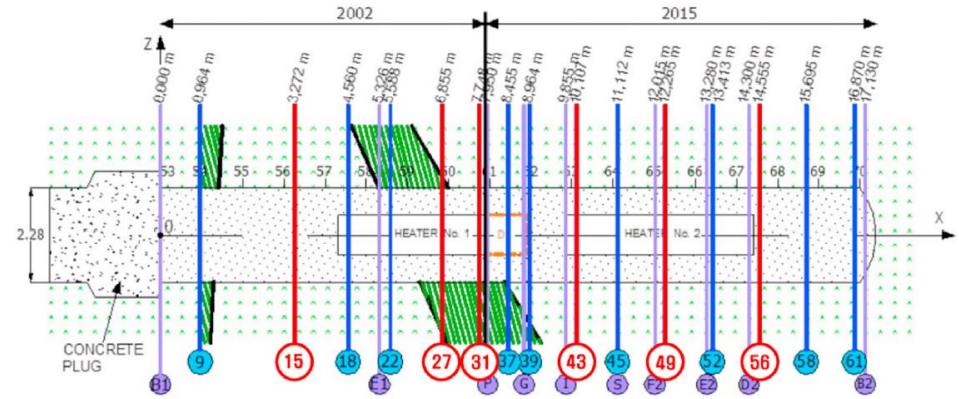
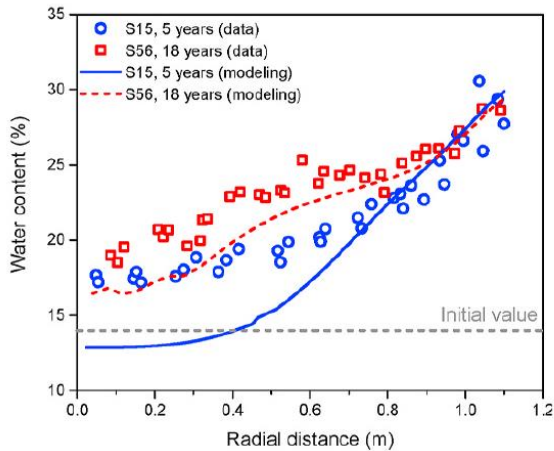
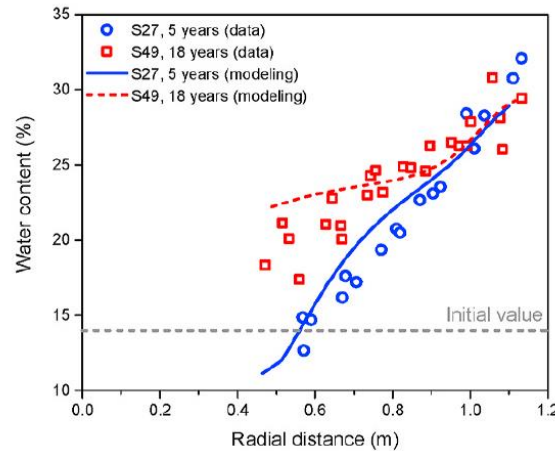


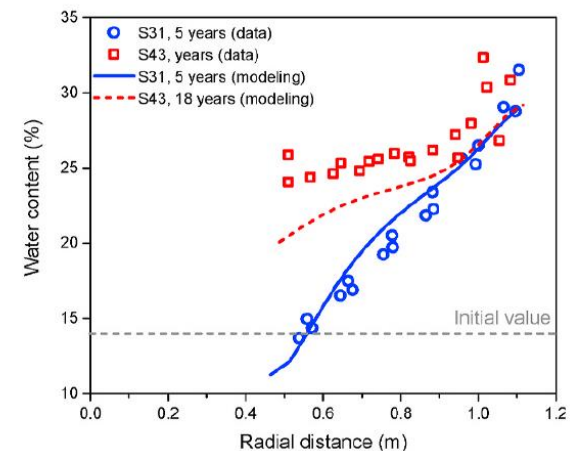
Fig.9. Location of sampling after dismantling sections



(a). Sections 15 and 56



(b). Sections 27 and 49



(c). Sections 31 and 43

# FEBEX test

## Dry density

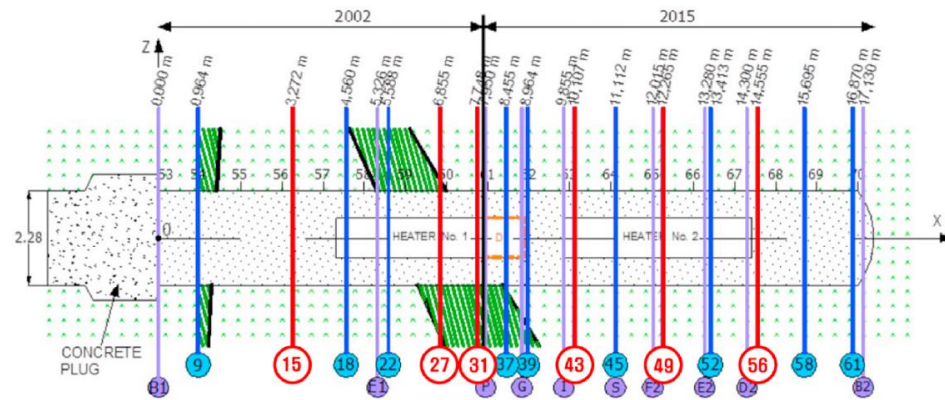
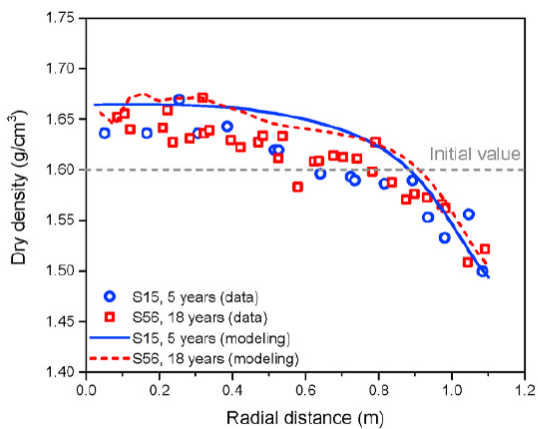
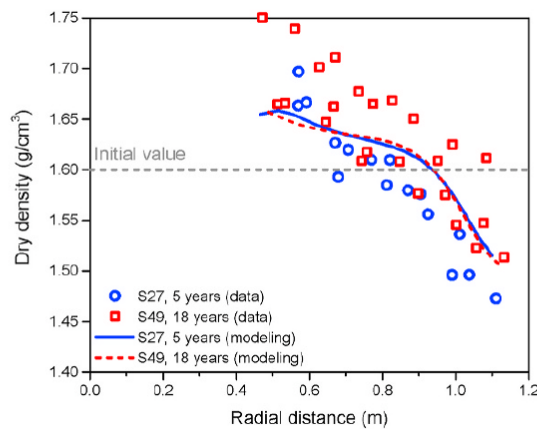


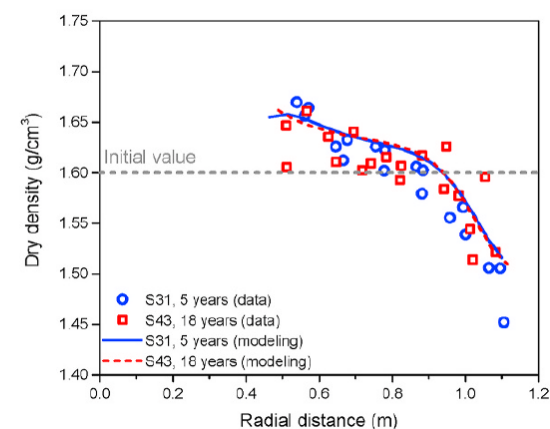
Fig.9. Location of sampling after dismantling sections



(a). Sections 15 and 56



(b). Sections 27 and 49



(c). Sections 31 and 43

# Conclusions



## Conclusions

- The numerical models in TOUGH2-MP/FLAC3D were able to **reproduce the coupled HM and THM behavior** at two in-situ experiments.
- The low dry density at the lower corner was not numerically observed, may be required to enhance and improve the models for better predictions.
- The difference between the power values measured in two heaters could not be simulated, taking into account the installation process at FEBEX and at least two types of rock masses, granite and lamprophyre.



—— Thank you for your attention. ——