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Supplement of

International collaboration in disposal research: comparative modeling of coupled processes in the DECOVALEX project

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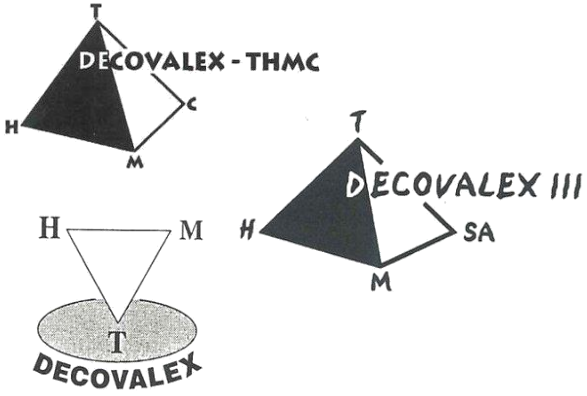

DECOVALEX 2023

DECOVALEX 2011 DECOVALEX 2015 DECOVALEX 2019

International Collaboration in Disposal Research:

Comparative Modeling of Coupled Processes in the DECOVALEX Project

Jens Birkholzer[1] and Alex Bond[2]

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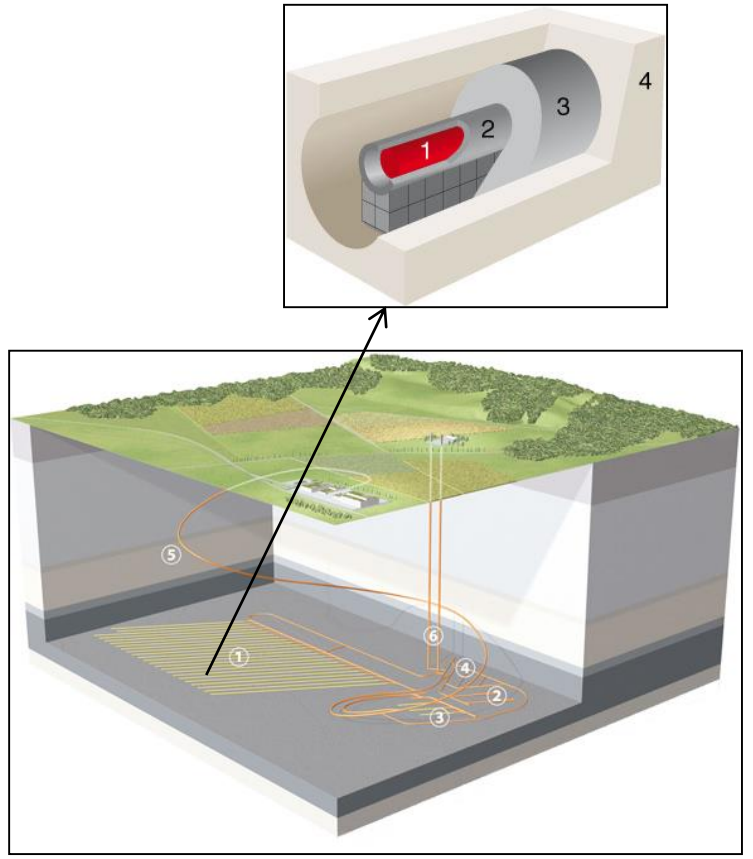
2) Quintessa Ltd., United Kingdom

SafeND – Interdisciplinary Research Symposium, November 10-12, 2021

The International DECOVALEX Project

DECOVALEX (acronym for DEvelopment of COupled models and their VALidation against EXperiments)

- DECOVALEX started in 1992 and has been going on ever since in separate 4-year stages
- Typically, in each phase, about 15 organizations and tens of research teams participate
- Focus is on THM/THMC couplings of key importance for deep geological disposal and other geosciences fields
- Research teams evaluate model results in comparison with other teams and against well designed field and laboratory experiments

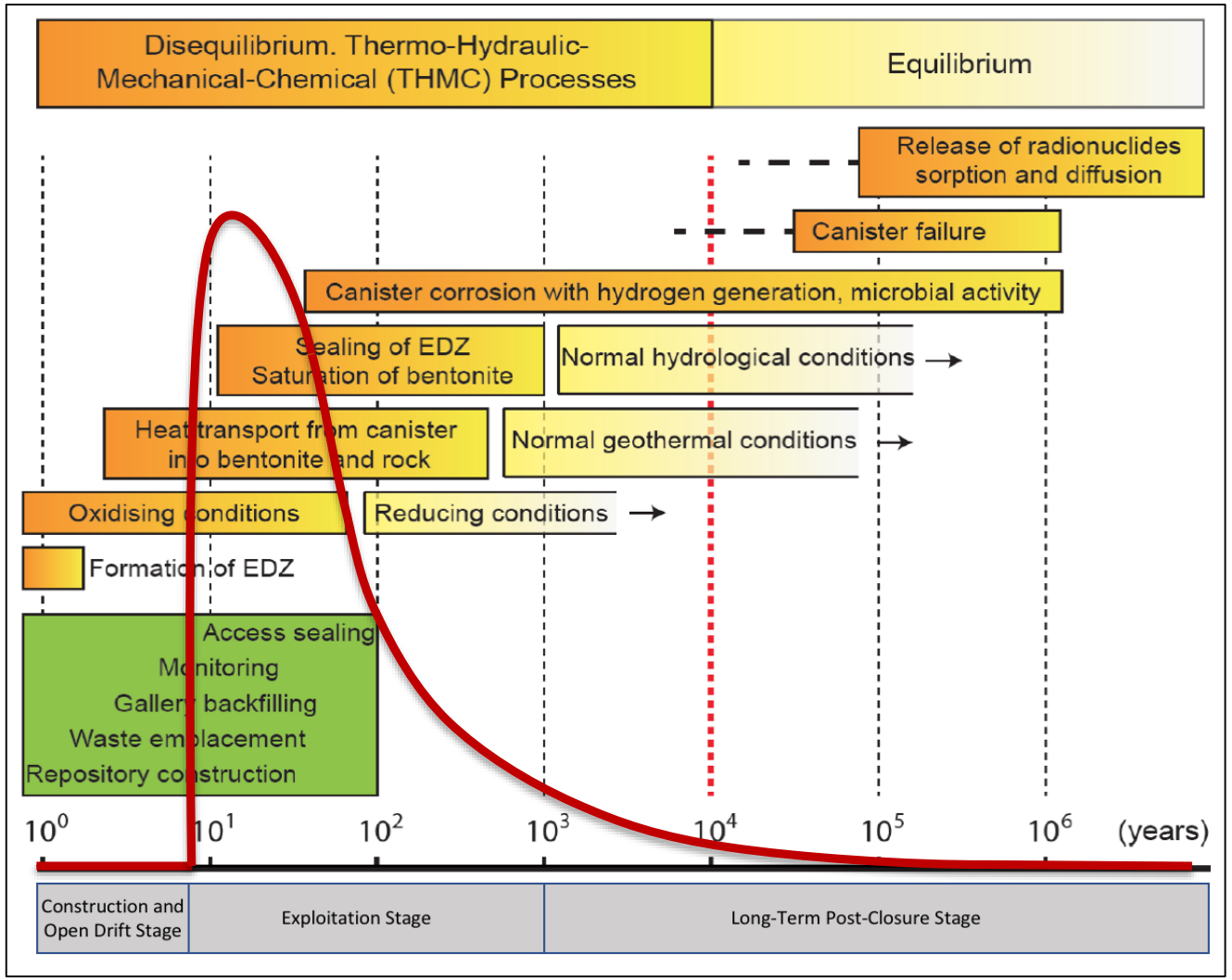


NAGRA, 2002

Coupled Processes and Performance Impact

- Excavation of tunnels changes stress field in the surrounding rocks
- Tunnel opening causes drying on tunnel walls and oxidizing conditions in rock
- Waste emplacement causes heat transport into bentonite and host rock
- Emplacement of bentonite initiates complex hydration processes
- Bentonite swelling provides pressure on tunnel walls
- Emplacement of engineered materials causes geochemical perturbations
- Gas generation causes pressure buildup and gas transport

RADIONUCLIDE TRANSPORT AND DOSE CALCULATIONS

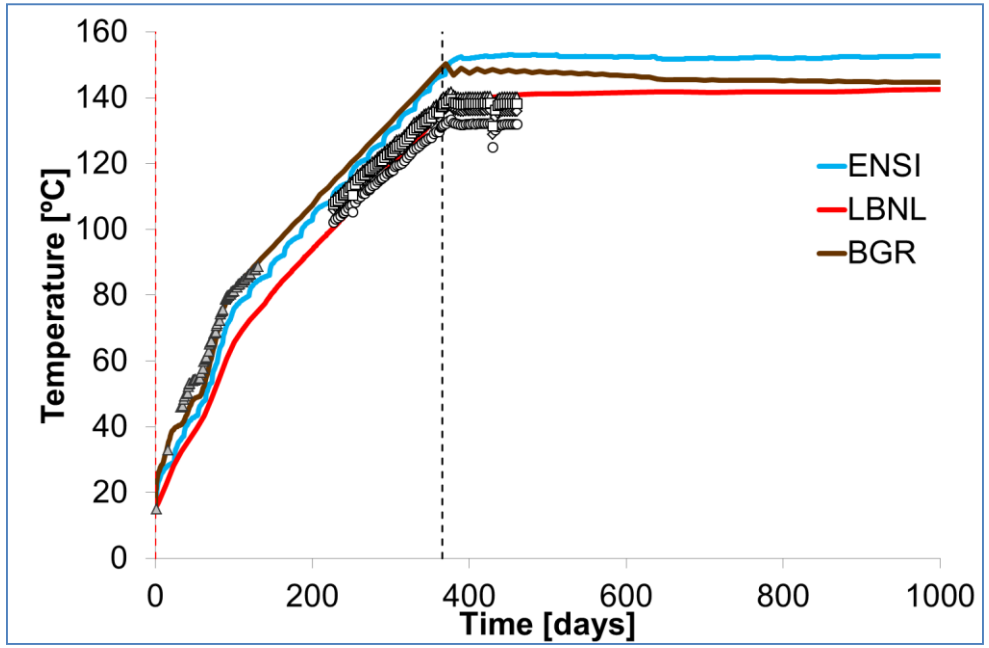


Modified from Bossart et al. (2017)

Typical DECOVALEX Collaboration Mode

Advanced experiments

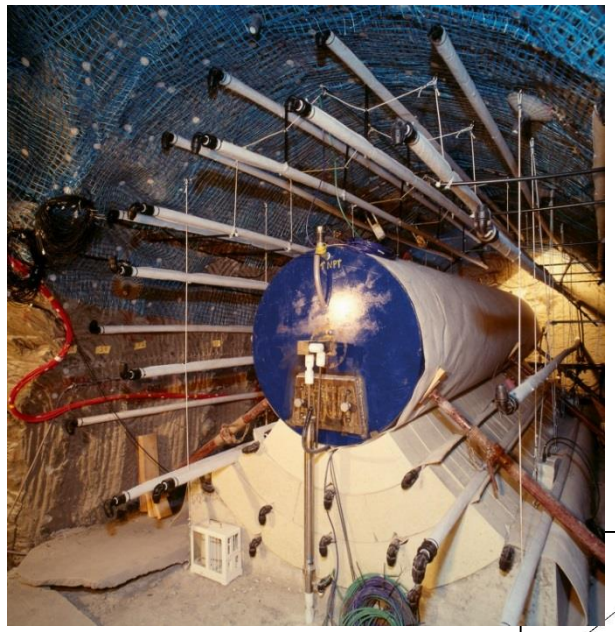
Team	Person	F.O.	Country	Code
BGR	Wang Xuerui	BGR	Germany	OpenGeoSys
CAS	Pengzhi Pan	CAS	China	EPCA3D
LBNL	Jonny Rutqvist	DOE	USA	TOUGH-FLAC
ENSI	Bastian Graupner	ENSI	Switzerland	OpenGeoSys
CNSC	Son T. Nguyen	IRSN	Canada/France	COMSOL
JAEA	Keisuke Maekawa	JAEA	Japan	THAMES
KAERI	Changsoo Lee	KAERI	South Korea	FLAC
CNWRA	Chandrika Manepally	NRC	USA	FLAC-xFlo

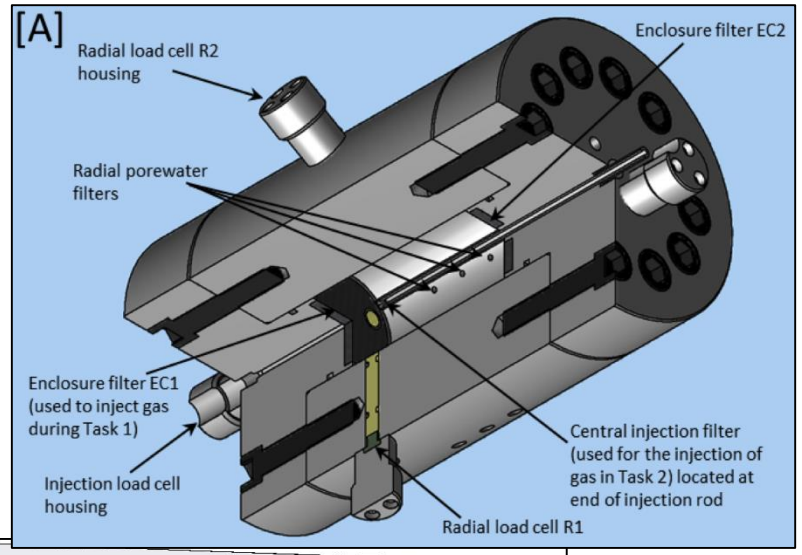


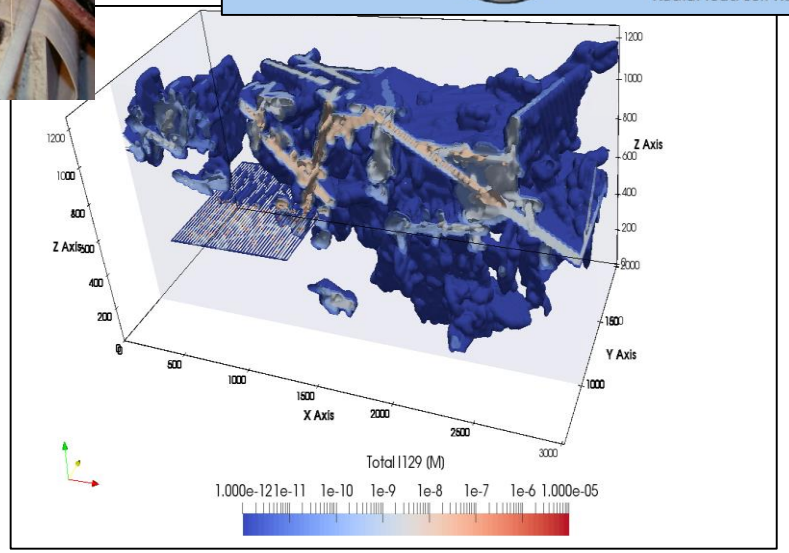
Detailed comparison with data

Various teams with various models

Typical DECOVALEX Modeling Tasks







Many tasks are aligned with major field experiments in underground research laboratories (URLs), often complemented by lab tests

Some tasks are hypothetical problems used for investigating specific modeling challenges, extrapolations over time, or performance evaluations

Tasks are proposed and defined according to the interests of participating organizations

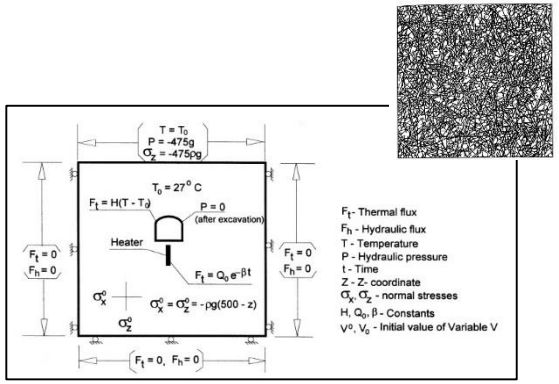
Tasks often involve modeling steps of increasing complexity

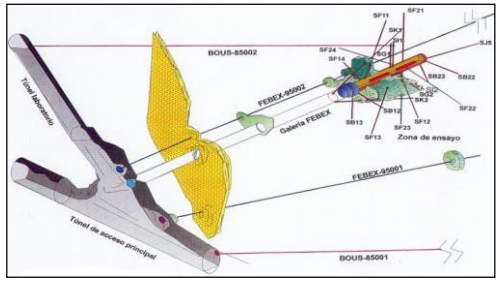
DECOVALEX Philosophy

- In-depth and regular in-person discussions among international organizations & research teams with different views
- Multiple approaches, conceptual models, and simplifications applied to the same problem
- A variety of challenges, designs, host rocks, processes
- Emphasis on comparative analyses
- Four-year project phases to provide ample time for team building and scientific progress
- Emphasis on information and knowledge exchange

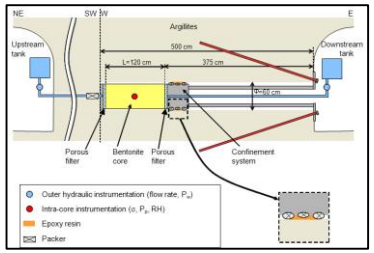
DECOVALEX Emphasis from 1992 Till Now

Initial focus: Coupled HM and THM Processes in Fractured Hard Rock

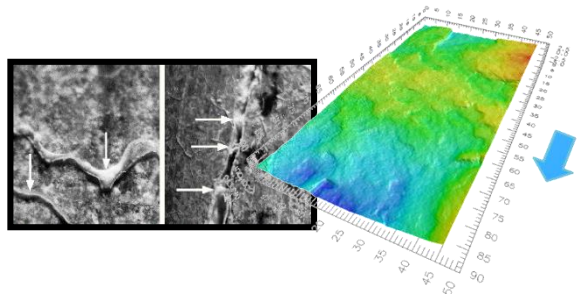




First Full-Scale THM Experiments in URLs



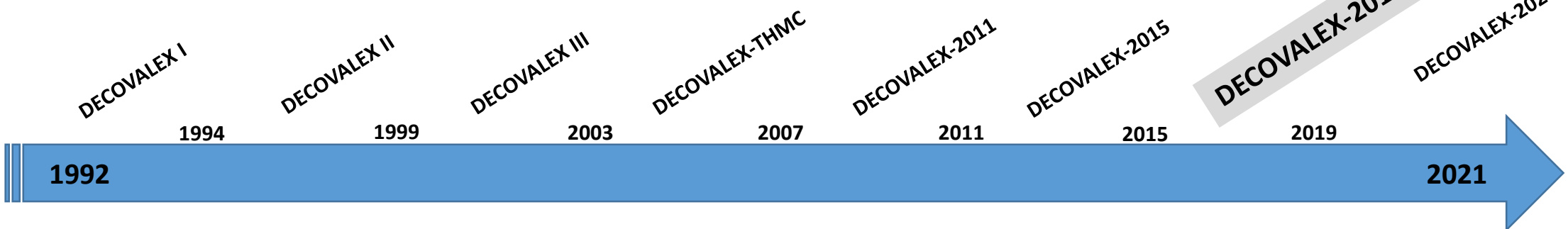
Added Emphasis on Clay- or Mudstone Host Rock and Bentonite Behavior



Adding Chemistry to THM

Broad Task Portfolios

- Multiple Host Rocks
- Engineered Barriers
- Safety Assessments
- Fundamental to Applied
- Beyond Nuclear Waste



DECOVALEX-2019 Phase: Seven Tasks

Fundamental Understanding of Processes

- Migration of gas in bentonite, led by BGS (UK)
- Fluid inclusions in salt, led by BGR (Germany)

THM Processes in Clay-Based Materials

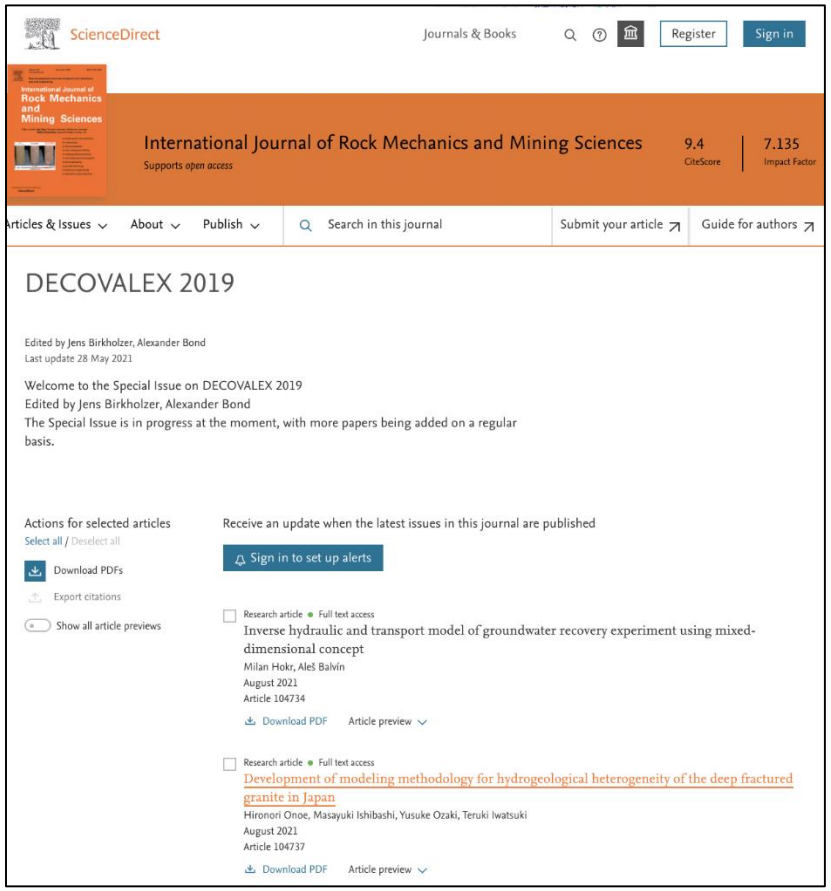
- Bentonite hydration & homogenization, led by UPC (Spain)
- Multi-scale THM processes in clay, led by Andra (France)

Modeling of Complex Fracture Systems

- Groundwater recovery in crystalline rock, led by JAEA (Japan)
- EDZ evolution in crystalline rock, led by SSM (Sweden)

Cross-Cutting Topic Beyond Nuclear Waste

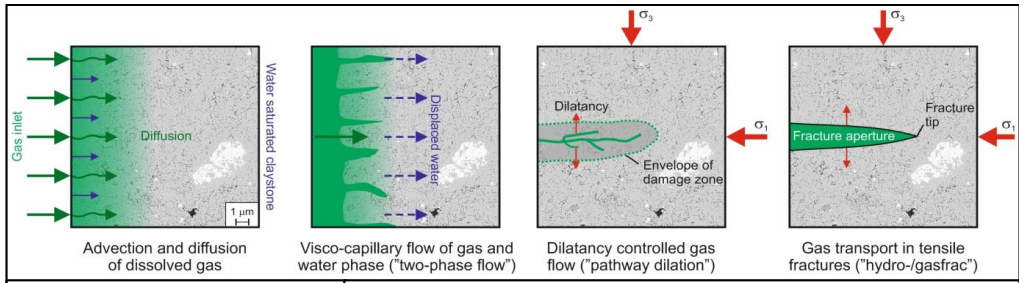
- Fault Slip Experiments, led by ENSI (Switzerland)



Virtual Special Issue on DECOVALEX-2019 in IJRMMS contains 29 related publications:
https://www.sciencedirect.com/journal/international-journal-of-rock-mechanics-and-mining-sciences/special-issue/10RM99KRN7V

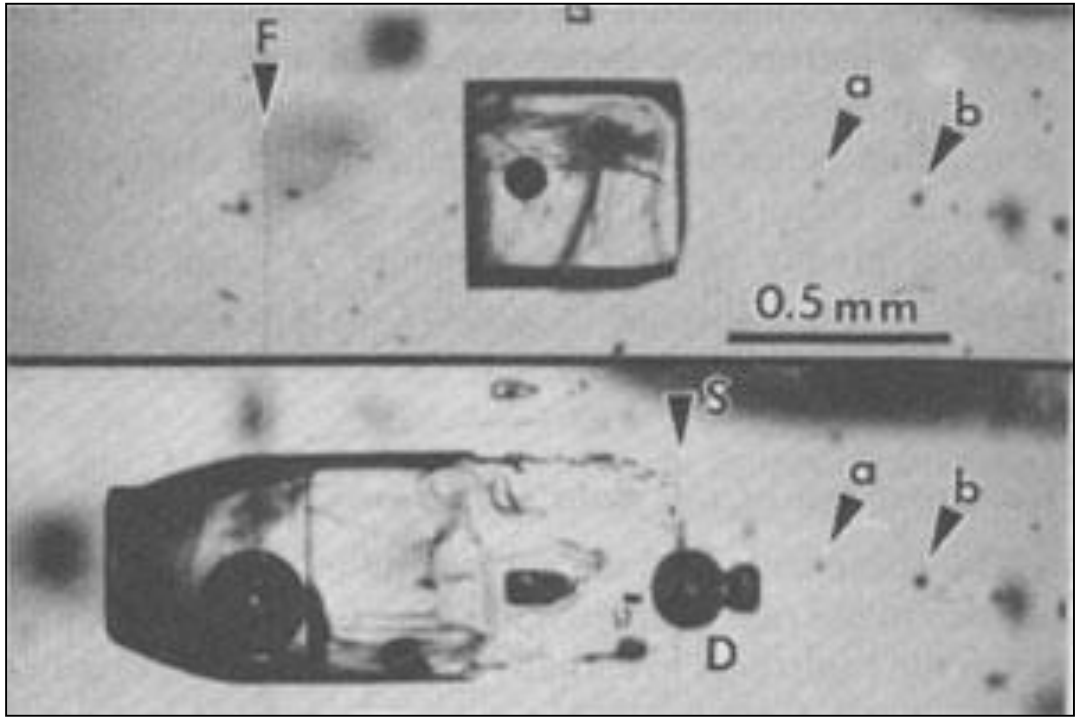
Fundamental Understanding of Processes

Advective Migration of Gas in Clays (7 teams)



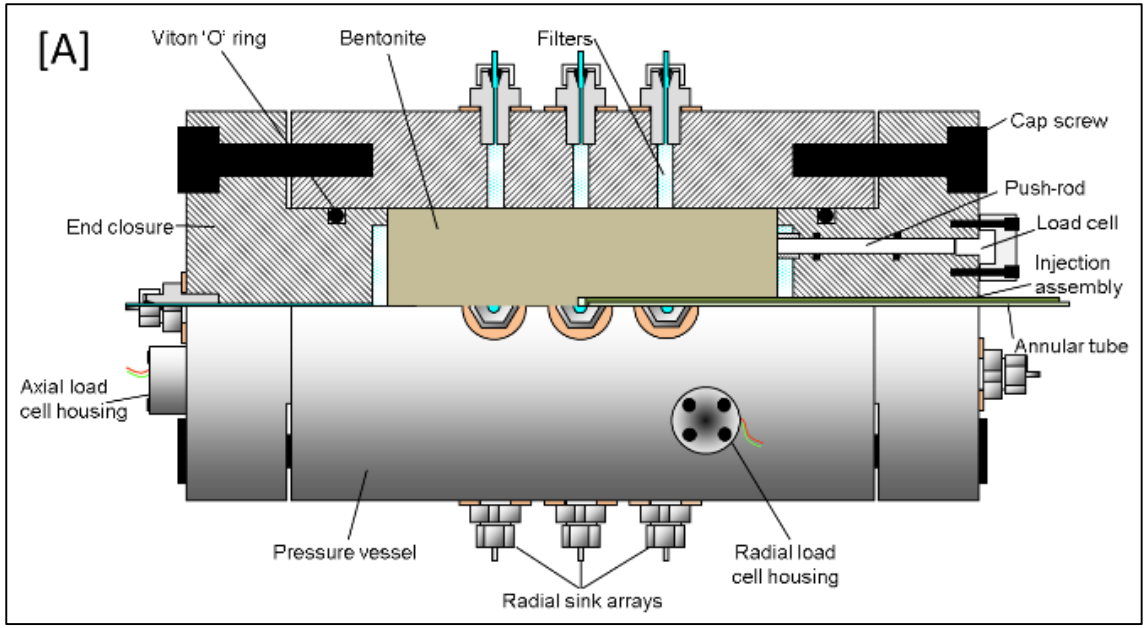
- This HM modeling task uses lab experiments exhibiting highly non-linear gas migration in bentonite
- Wide range of continuum and discrete models applied
- HM models with implicit or explicit consideration of pathway dilation work well

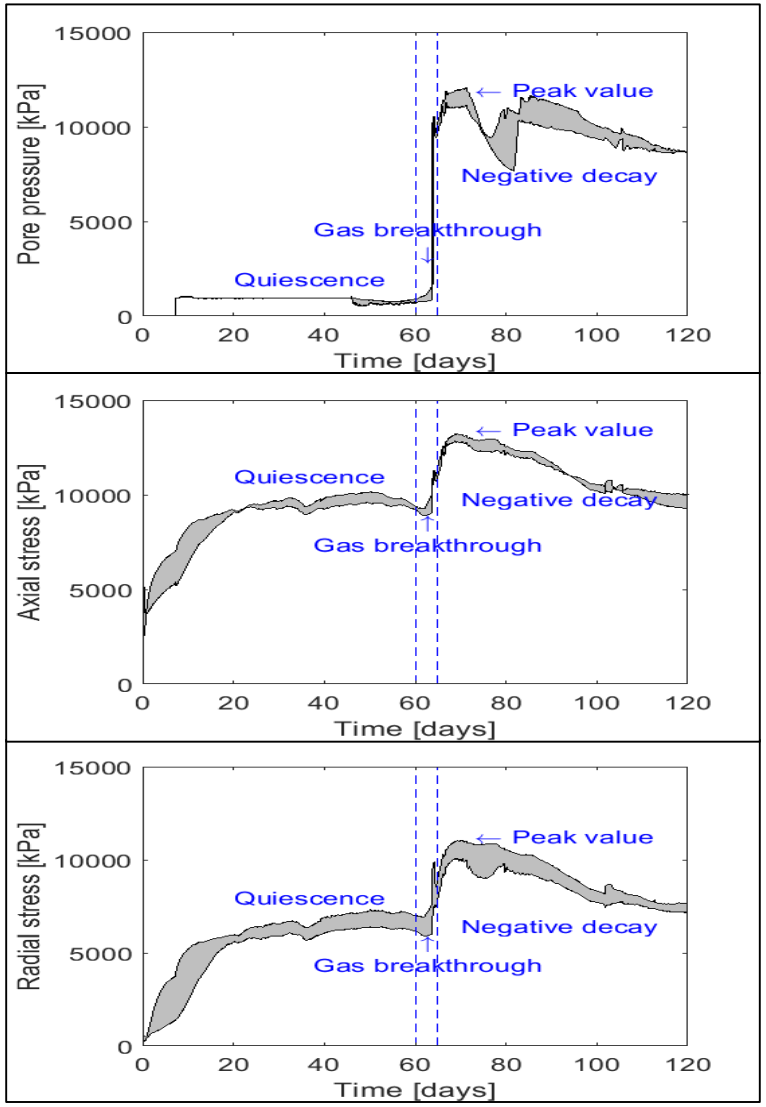
Fluid Inclusions in Salt (3 teams)



- High fluid inclusion pressure at the halite-grain boundaries can cause dilating flow pathways
- Liquid fluid inclusions in salt can move towards a heat source as a result of directional dissolution
- Micro-scale controls need to be explicitly modeled

Gas Migration: Test Design and Data





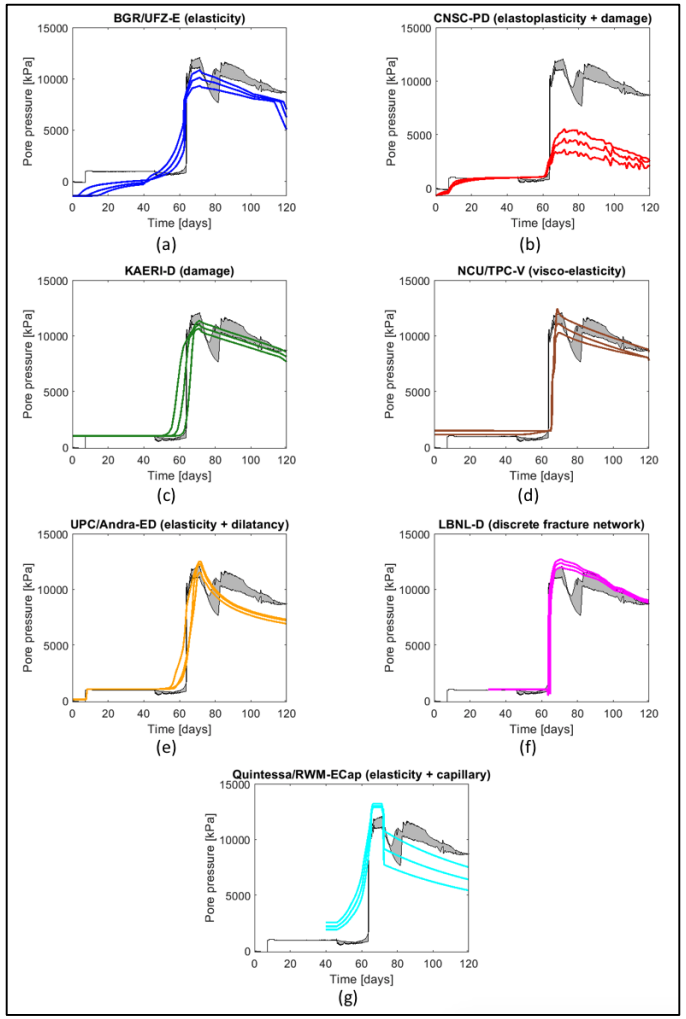
Gas Migration: Model Approaches and Codes

- Standard two-phase flow continuum models incorporating a range of mechanical deformation behaviors
- Enhanced two-phase flow models with pathways embedded in a plastic material (continuous techniques)
- Enhanced two-phase flow models with pathways generation via rigid-body-spring network (discrete approaches)
- Single-phase gas flow models with a creep damage function
- Nonlinear gas bubble transport model with pressure-induced dilation

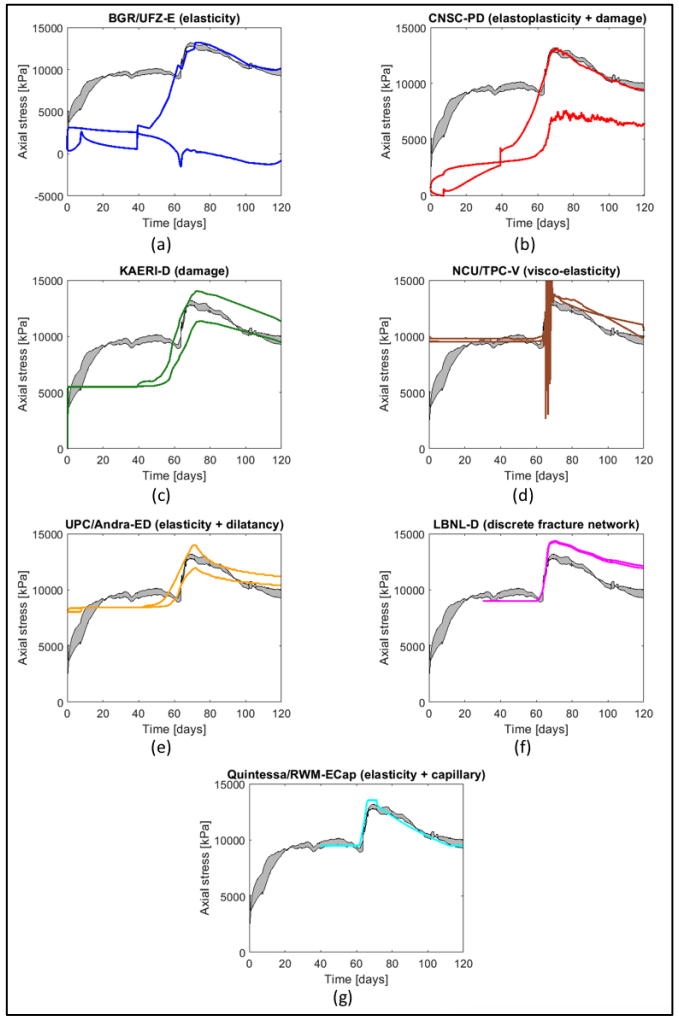
Model	Funding Organization	Code	Kind of model	Mechanical deformation	Hydraulic approach
BGR/UFZ-E	BGR/UFZ	OpenGeoSys	continuous	elasticity	two phases
CNSC-PD	CNSC	COMSOL Multiphysics®	continuous	elastoplastic damage	two phases
KAERI-D	KAERI	Stage 1: TOUGH2 / FLAC3D Stage 2: COMSOL Multiphysics®	continuous	elastic damage model	two phases
NCU/TPC-V	Taiwan Power Company	THMC	continuous	visco-elastic	two phases
CIMNE-UPC/ Andra-ED	ANDRA	Code_bright	continuous	elasticity with dilatancy	two phases with embedded fracture
LBNL-D	US DOE	TOUGH-RBSN	discontinuous	elastic-brittle damage and fractures	two phases
Quintessa/ RWM-ECap	RWM	QPAC	continuous	elasticity	single phase

Gas Migration: Model Comparison

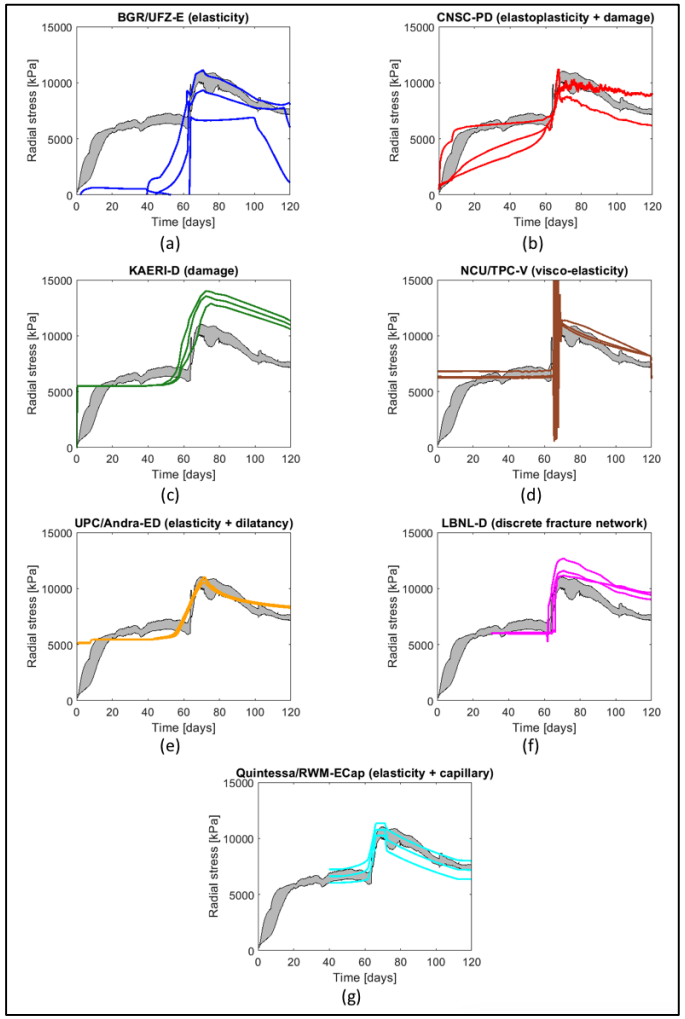
Pore Pressure



Axial Stress

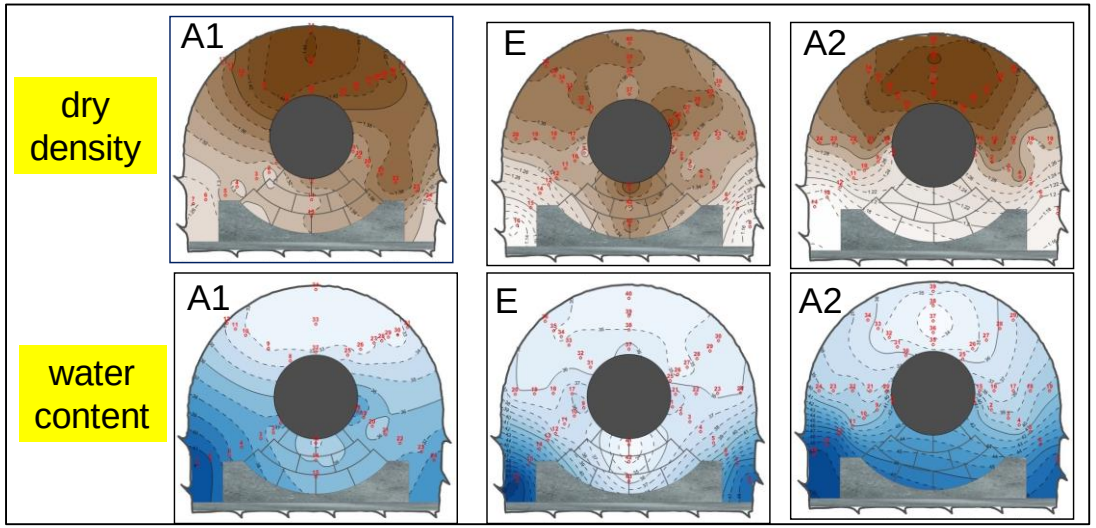


Radial Stress



THM Processes in Clay-Based Materials

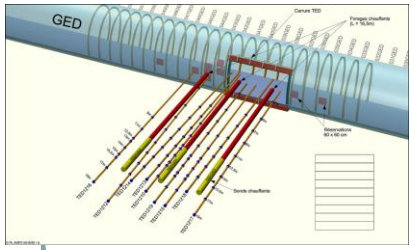
Bentonite Hydration and Homogenization (4 teams)



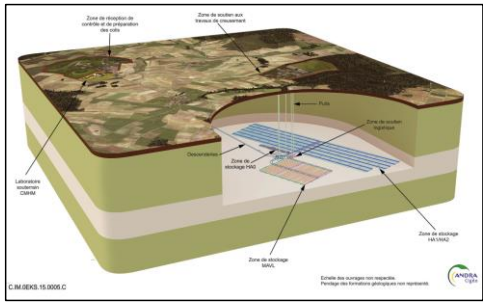
- Task involved modeling of hydration and homogenization using the EB (HM) and FEBEX *in-situ* experiments (THM) at, respectively, Mont Terri and Grimsel test Site
- Modeling teams obtained good representation of the measured thermal and hydrological evolution of the hydrating bentonite barrier
- Representation of the plastic deformation and homogenization of the bentonite remains challenging

Multi-scale THM Processes in Clay (5 teams)

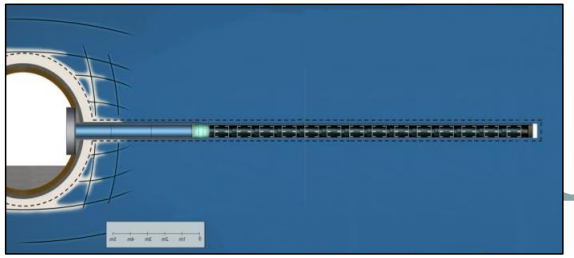
Small-scale TED Experiment



Repository Scale



Full-scale ALC Experiment

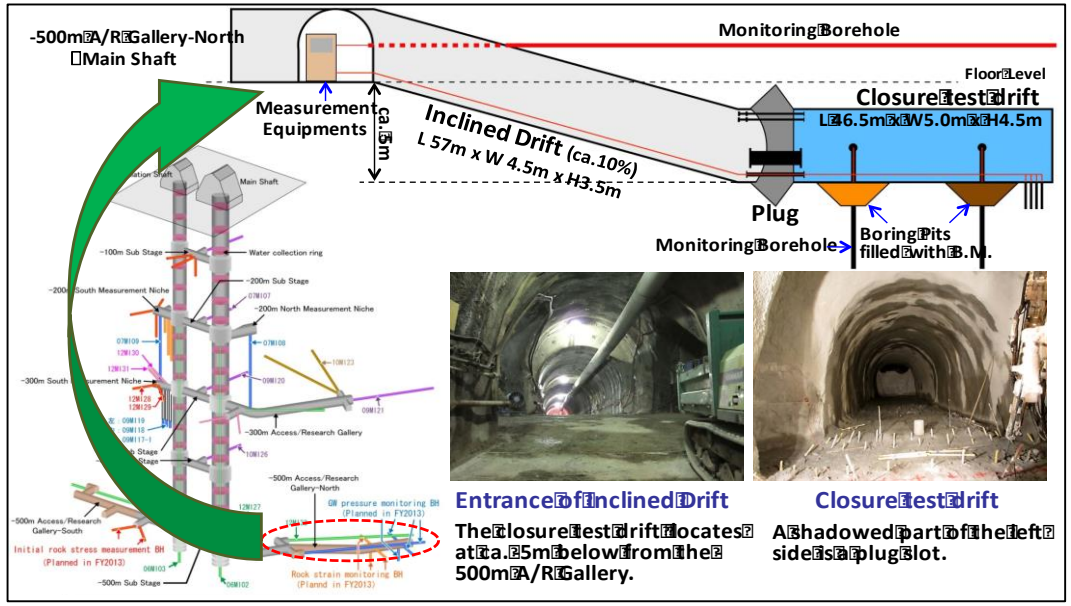


Tests at Bure URL, led by ANDRA

- Thermo-poro-elastic models yielded good representation of the two *in-situ* heating experiments at the Bure URL, including upscaling from the TED to the ALC tests
- A broad range of modeling approaches was applied to the repository modeling task, leading to a set of best practices guidelines for repository-scale modeling

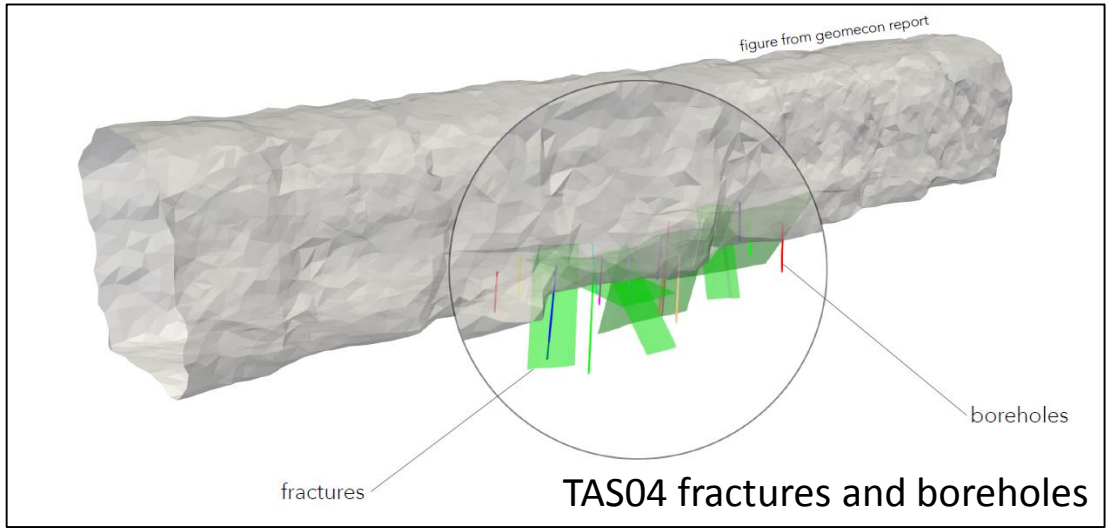
Modeling of Complex Fracture Systems

Groundwater Recovery in Crystalline Rock (3 teams)



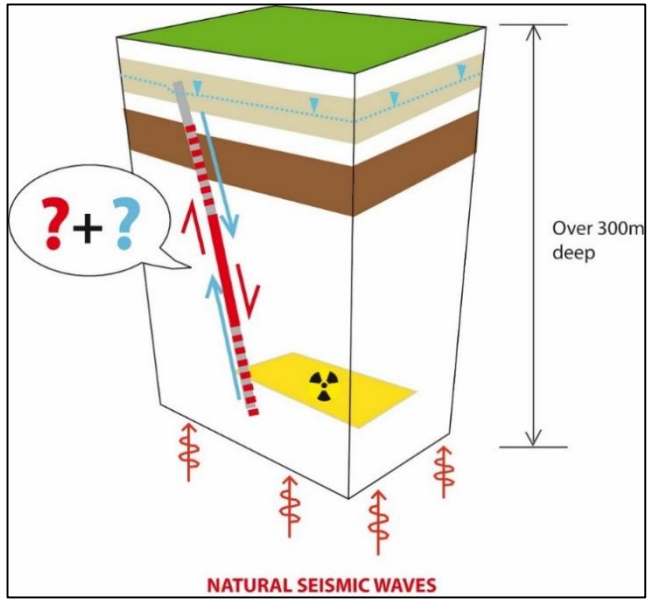
- Task involved modeling the hydraulic, mechanical, and chemical response to flooding of the GREET tunnel
- A combined stochastic and deterministic approach with high permeability fractures represented well the inflow into the tunnel, hydraulic drawdown and recovery
- Variation of Cl concentration around the tunnel was very difficult to reproduce

EDZ Evolution in Crystalline Rock (3 teams)



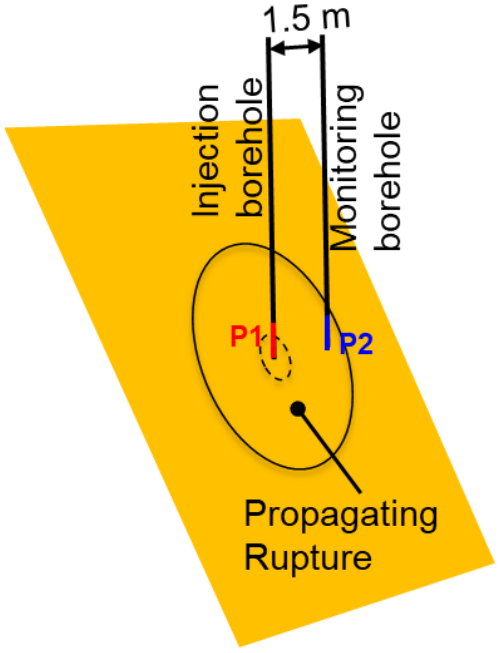
- Task aimed at understanding the permeability changes due to formation of an excavation damage zone (EDZ), based on the TAS04 tunnel EDZ experiment in the Äspö HRL
- Modeling teams got overall trends right, but were not able to match all details of interference tests conducted to measure EDZ properties
- Channelization within the fracture network could be the cause of the difficulties in modeling the observations

Complex HM Processes with Relevance Beyond Nuclear Waste: Fault Reactivation (6 teams)



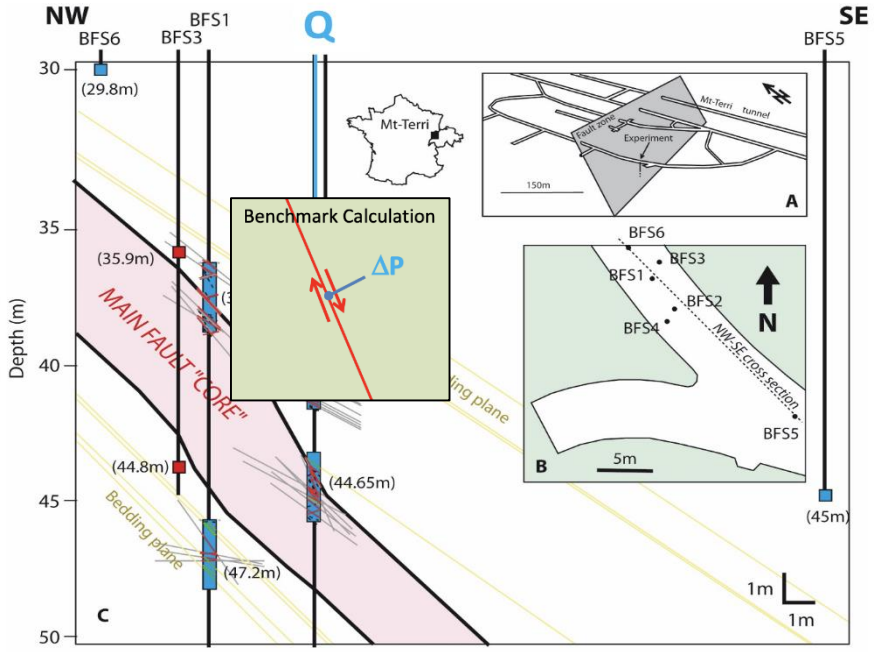
Fault Slip and Permeability Creation Due to Repository-Induced Perturbation

- Fluid or Gas Pressure Buildup
- Triggering from Distant Earthquakes



Hydromechanical Fault Models Using

- Interfacial Fault Models
- Solid Element Fault Models
- Different Fault Permeability Concepts



Mont Terri Fault Slip (FS) Experiment

- Controlled injections into fault zone
- High-resolution monitoring of flow rate, fault deformation, and seismicity

- Initial benchmarking exercise provided coherence between the modeling tools
- Both interfacial and solid-element fault models were appropriate, provided they allowed for abrupt permeability increase
- Differences remain in more complex cases where plastic damage on shear features plays an important role

29 Years of DECOVALEX: Achievements

- DECOVALEX has addressed a wide range of issues related to engineered and natural system behavior in argillaceous, crystalline and other host rocks
- DECOVALEX has yielded in-depth knowledge of coupled THM and THMC processes associated with nuclear waste repositories and other geo-applications
- DECOVALEX has advanced the capability, as well as demonstrated the suitability, of numerical simulation models for quantitative analysis
- DECOVALEX has evaluated, and reduced, model uncertainty stemming from conceptual model choices
- Results have been published in books, numerous journal articles (e.g., including several Special Issues), and conference proceedings
- Many doctoral students and other early-career researchers have participated as members of research teams to the project

Planning for next DECOVALEX Phase (D-2027) will start next year

Thanks to our 17 Partner Organizations

Backup Slides

DECOVALEX-2023: Themes and Tasks

Understanding of Processes and Impact on Safety

- SAFENET: Micro-Scale THMC Lab Experiments with Focus on Shear
- Modeling Advection of Gas in Clays (MAGIC)
- Heat and Gas Fracturing in Clays (HGFrac)

Full-Scale THM Demonstration Experiments

- THM Modeling of the FE Experiment
- Full-scale Engineered Barrier System Experiment at Horonobe URL

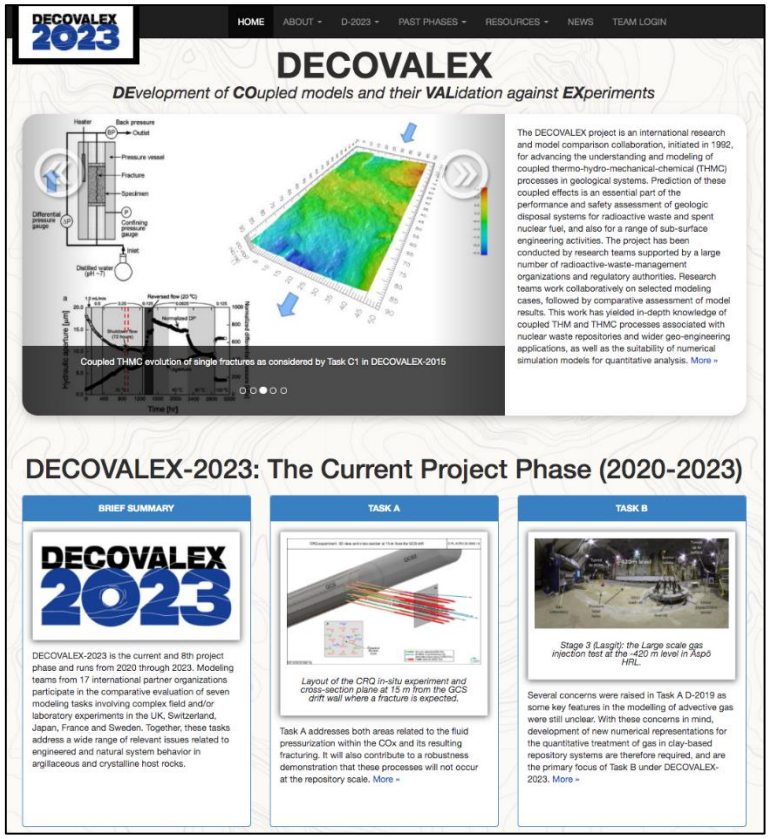
THM Behavior of Salt as a Host Rock

- Brine Availability Test in Salt (BATS)

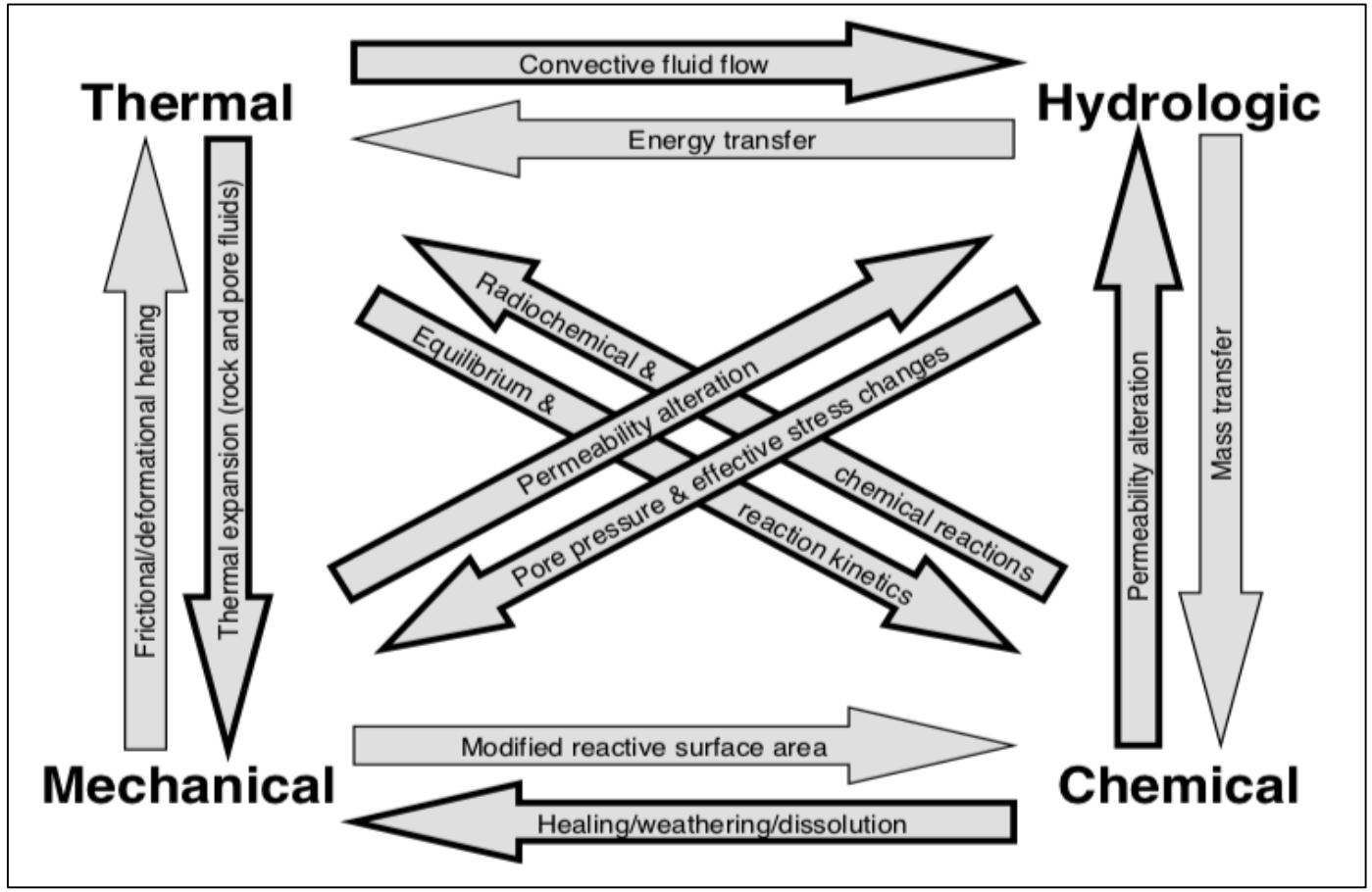
Performance Assessment (PA) Methodologies

- Comparison of PA Methods for Two Generic Repository Cases

More Info at www.decovalex.org



Coupled THMC Processes Relevant to Disposal



From Yow and Hunt et al. (2012)

Modeling Challenges

- THMC processes are highly nonlinear and involve steep gradients
- They have widely different time and spatial scales
- Constitutive relationships are complex and often contain hard-to-measure parameter sets
- Various numerical method exist for solving THMC processes, each with their own merits and disadvantages