MODELLING OF THE LONG-TERM EVOLUTION AND PERFORMANCE OF ENGINEERED BARRIER SYSTEM

A joint ACED, BEACON, DONUT & MAGIC contribution

F. CLARET, A. DAUZERES, D. JACQUES, P. SELLIN

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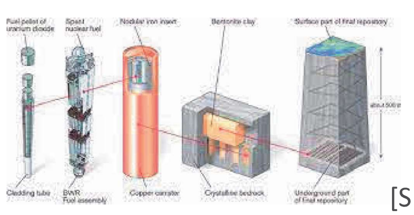
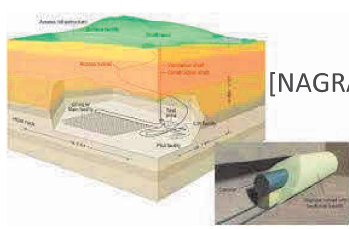
CONTEXT: A MULTI-BARRIER SYSTEM OF ENGINEERED (NEAR FIELD) AND NATURAL BARRIERS (NEAR AND FAR FIELD) IS FORESEEN IN MOST OF THE REPOSITORY DESIGNS

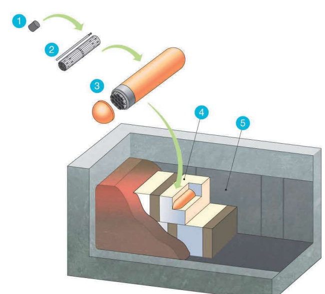


[SKB]



[NAGRA]

P. SELLIN and O.X. LEUPIN Clays and Clay Minerals, Vol. 61, No. 6, 477–498, 2013.



[NWMO]

https://www.nwmo.ca/en/

- The Engineered Barrier System (EBS) itself comprises a variety of components, such as the waste form itself, waste canisters, backfill, seals, and plugs.
- Materials, designs and safety functions of the EBS depend on the host rock and the concept developed in each country.

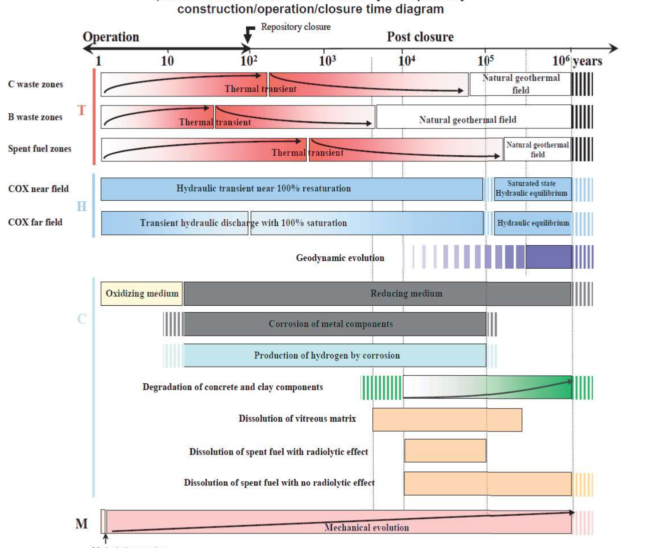
CONTEXT: A LINK TO EURAD SRA THEME 3 ENTITLED "ENGINEERED BARRIER SYSTEM PROPERTIES, FUNCTION AND LONG-TERM PERFORMANCE"

A list of RD&D priorities and activities of common interest to be addressed within EURAD for theme 3 have been established. Amongst others, the following priorities have to be considered:

- Improved understanding of the interactions occurring at interfaces between different barriers including waste packages in the disposal facility.
- Characterized bentonite / clay-based material evolution under specific conditions to provide data on hydro-mechanical, thermal and chemical behavior
- Improved quantification and understanding of cement-based material evolution to improve long-term modelling and assessments.
- Improved understanding of the performance of plugs and seals
- Improved description of the spatial and temporal evolution of transformations affecting the porous media and degrading materials in the near field of HLW and ILW disposal systems.

EBS PROPERTIES WILL EVOLVE WITH TIME IN RESPONSE TO THE THERMAL, HYDRAULIC, MECHANICAL, RADIOLOGICAL AND CHEMICAL GRADIENTS AND INTERACTIONS BETWEEN THE VARIOUS CONSTITUENTS OF THE BARRIERS AND THE HOST ROCK

Figure 1. **Chronogram of the major phenomena affecting the repository and its geological environment (based on the conventional hundred-year repository construction/operation/closure time diagram)**



Modified from Plas, F. and P. Landais (2008). "The Phenomenological Analysis of Repository Situations (PARS) -Application within the dossier 2005 ARGILE (Meuse/Haute-Marne site)." Safety Cases for Deep Geological Disposal of Radioactive Waste: Where Do We Stand?: 203 -210

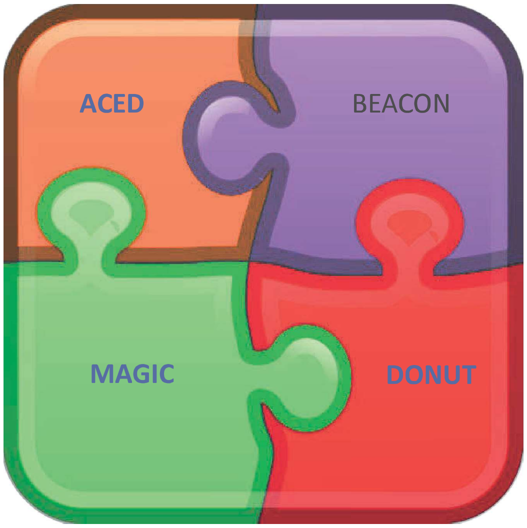
- THMCR Coupled phenomena
  - Weak/strong
  - Time-varying
- Many time and space scales to manage
  - > 10 orders of magnitude in time scale
  - From operating period to post-closure period (1 Myears)

Assessing how the EBS properties evolve over long time frames is highly relevant for evaluating the performance of a repository systems and for evaluation of its safety functions in a safety case.

- For this purpose, mechanistic numerical models are increasingly being used
- Such models provide an excellent way for integrating in a coherent framework scientific understanding of coupled processes and their consequences on different properties of the materials in the engineered barrier system

MODELLING OF THE LONG-TERM EVOLUTION AND PERFORMANCE OF ENGINEERED BARRIER SYSTEM

a joint effort and a shared goal



MODELLING OF THE LONG-TERM EVOLUTION AND PERFORMANCE OF ENGINEERED BARRIER SYSTEM

F. CLARET[1], A. DAUZERES[2], D. JACQUES[3], P. SELLIN[4], B. COCHEPIN[5], L. DE WINDT[6], J. GARIBAY-RODRIGUEZ[7], O. LEUPIN[8], A. MON LOPEZ[9], L. MONTENEGRO[9], V. MONTOYA[7,3], N. PRASIANAKIS[10], J. SAMPER[9], J. TALENDIER[5]

[1]BRGM, 3 avenue Claude Guillemin 45060 Orléans, France, f.claret@brgm.fr

[2]IRSN, PRP-DGE/SRTG/LETIS, BP 17, 92262 Fontenay-aux-Roses Cedex, France, a.dauzeres@irsn.fr

[3]SCK CEN, Belgian Nuclear Research Centre,Institute for Environment, Health and Safety, Mol 2400, Belgium, diederik.jacques@sckcen.be; vanessa.montoya@sckcen.be

[4]SKB, Stockholm, Sweden Sweden, patrik.sellin@sk.se

[5] Andra, 1/7, rue Jean Monnet, Parc de la Croix-Blanche, 92298 Châtenay-Malabry Cedex France, benoit.cochepin@andra.fr; jean.talendier@andra.fr

[6] MINES ParisTech, PSL University, France, laurent.de_windt@minesparis.psl.eu

[7] UFZ, Helmholtz Centre for Environmental Research—UFZ/TU Dresden, Leipzig, Germany, jaime.garibay-rodriguez@ufz.de , vanessa.montoya@ufz.de

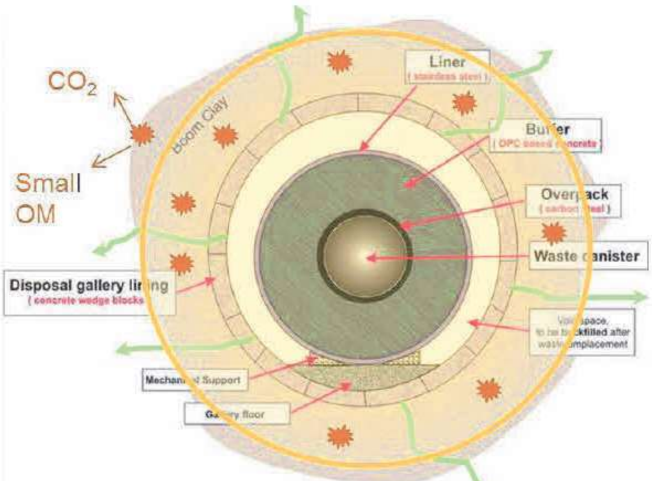
[8] NAGRA, Nagra Hardstrasse 73, Postfach 280,5430 Wettingen, Switzerland, Olivier.Leupin@nagra.ch

[9] UDC, Centro de Investigaciones Científicas Avanzadas (CICA), ETS Ingenieros de Caminos, Canales y Puertos, Universidade da Coruña, A Coruña Spain, alba.mon@udc.es, lmontenegro@udc.es, j.samper@udc.es

[10] Laboratory for Waste Management, Paul Scherrer Institut, 5232, Villigen, Switzerland, nikolaos.prasianakis@psi.ch

PROJECTS CONTRIBUTIONS TO THE SCIENTIFIC BASIS FOR EBS EVOLUTION AND MODELLING OF THEIR EVOLUTION

ACED – ASSESSMENT OF CHEMICAL EVOLUTION IN A ILW OR HLW DISPOSAL CELL



Maes (2014)

- **DISPOSAL CELL.**
  - Intermediate level waste package
  - High level waste package
  - Immediate host rock surrounding (clay, crystaline)
- **CHEMICAL EVOLUTION**
  - Different materials (glass, steel, different types of cement-based materials, host rocks)
  - Chemical gradients – Transport
  - Disequilibrium – Geochemical reactions
- **ASSESSMENT**
  - Large structures
  - Long times

ACED – ASSESSMENT OF CHEMICAL EVOLUTION IN A ILW OR HLW DISPOSAL CELL

Long term chemical evolution forms an important input for the assessment of the evolution of a disposal system and the assessment of safety- and performance-related aspects

AIM – A better conceptual and mathematical representation of the chemical evolution to:

- Improve the assessment and quantification of generic safety functions such as isolation and containment of waste constituents
- Obtain a better substantiation of conservatism and reduction of uncertainty
- Increase the scientific basis for definition of requirements of materials

OBJECTIVE – For the assessment of the chemical evolution at the disposal cell scale:

- Improve methodologies for deriving multi-scale quantitative models for assessment of chemical evolution
- Derive robust models (including key processes)

CHEMICAL EVOLUTION AT DIFFERENT SCALES

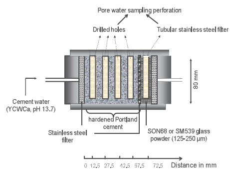
INTERFACE SCALE

WASTE PACKAGE SCALE

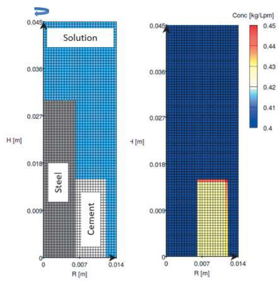
DISPOSAL CELL SCALE

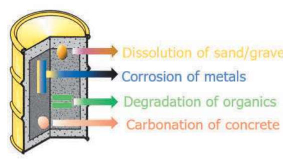
Experimental study

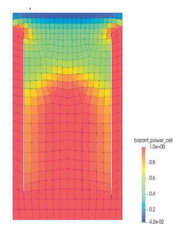
STEEL-CONCRETE and STEEL-CLAY

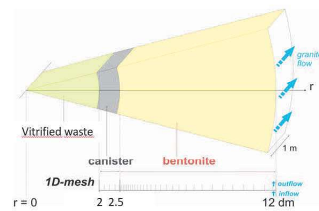


Numerical study – coupled reactive transport models

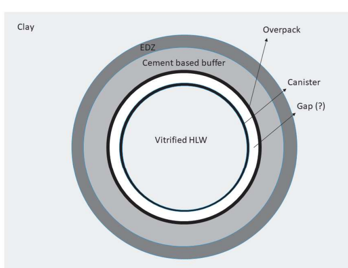


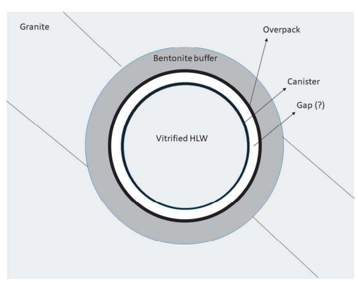




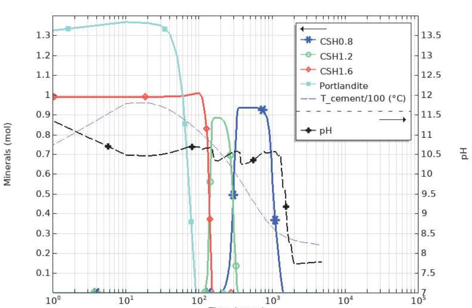


REPRESENTATIVE DISPOSAL CELLS - HIGH-LEVEL ACTIVE WASTE

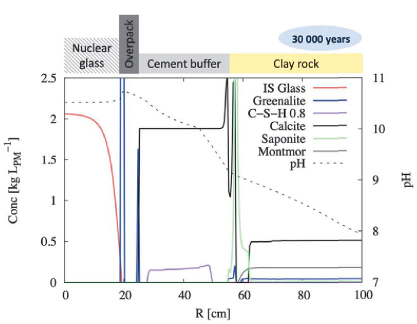


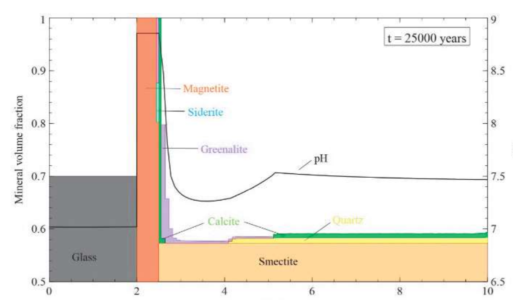


Modelling of the transient temperature stage in a HLW cell in clay with cement-based buffer

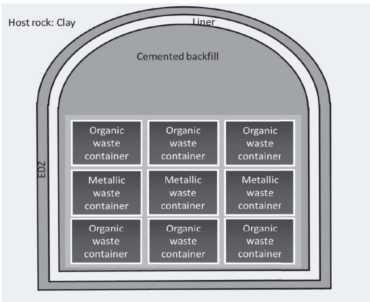


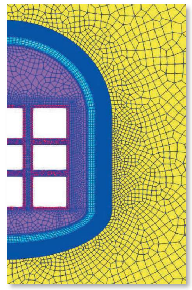
Modelling of the geochemical evolution in a HLW disposal cell in clay (HYTEC) and granite (CORE^{2D})

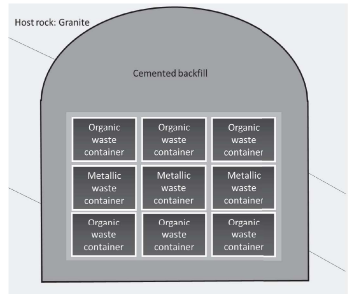




REPRESENTATIVE DISPOSAL CELLS – LOW-LEVEL ACTIVE WASTE

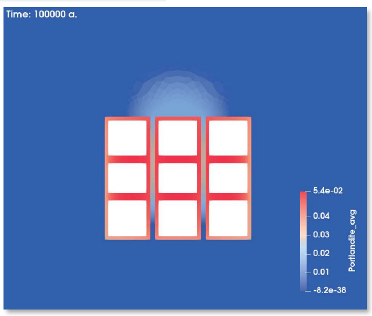


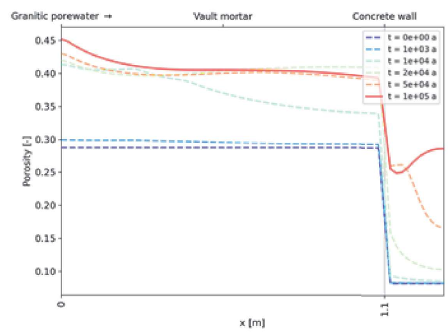




Porosity changes at different times along a horizontal profile (granite, code: OpenGeoSys)

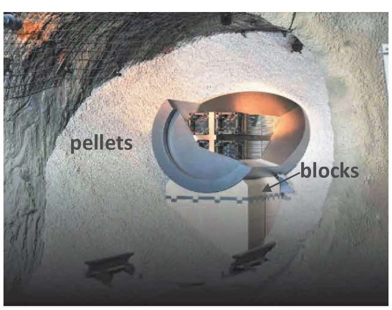
Portlandite distribution in clay rock (code: OpenGeoSys)

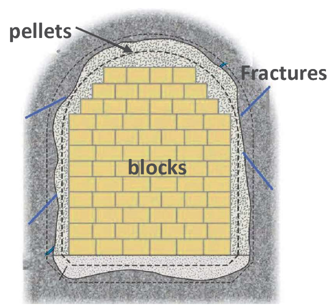




BEACON
Bentonite Mechanical Evolution

BEACON: BENTONITE ENGINEERED BARRIER MECHANICAL EVOLUTION EFFECTS ON THE LONG-TERM PERFORMANCE OF THE BARRIER





Bentonite is used as barrier around canister or to seal tunnels and shafts

Initial distribution of properties (dry density, water content…)
- Pellets mixtures
- Combination between blocks and pellets
- Joint between blocks
- Technological voids…

→ Initial heterogeneities

○ Bentonite materials are initially dry and will be saturated progressively with water coming from host rock

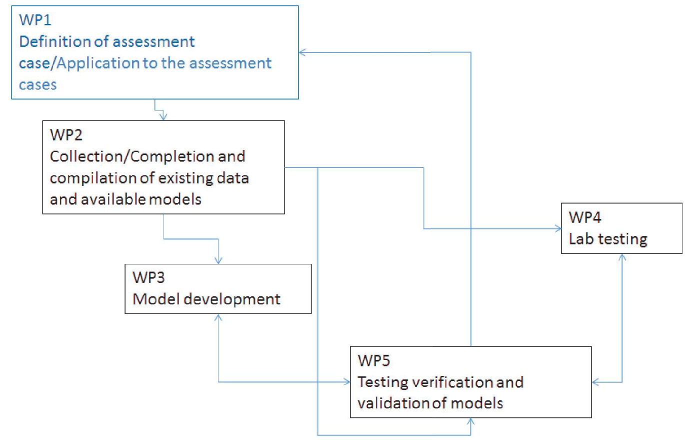
External solicitations
- Local water flow
- Stress field around the bentonite-based component
- Thermal distribution and evolution

→ induced heterogeneities

→ Need to model the hydromechanical evolution from installation to long term equilibrium including likely heterogeneities

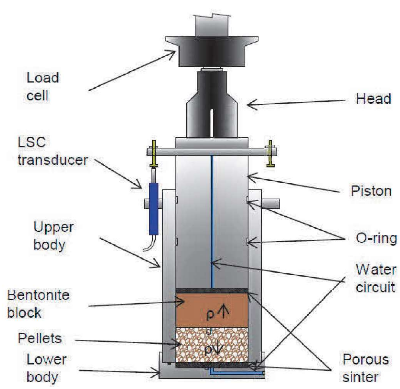
BEACON AT GLANCE

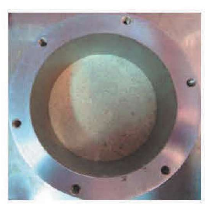
- Part of HORIZON2020
- Running 2017-2022
- Objectives:
  - To develop and test the tools necessary for the assessment of the mechanical evolution of an installed bentonite barrier
    - and the resulting performance of the barrier
  - To verify the performance of current designs for buffers, backfills, seals and plugs.
  - Beacon is focused on the direct application to real assessment cases in actual repository systems
    - cases from relevant repository systems have been selected as test examples



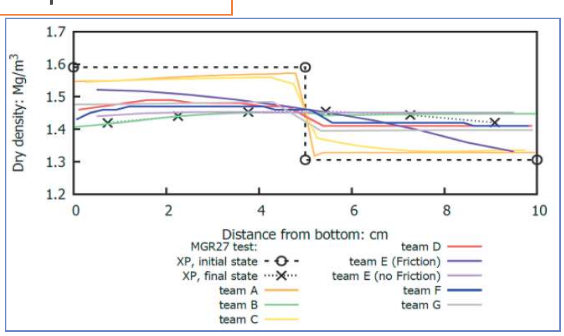
VALIDATION OF MODELS AGAINST EXPERIMENTS

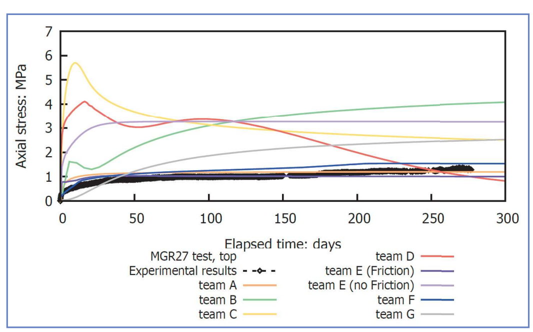
Experiment





Models: Blind prediction





BEACON
Bentonite Mechanical Evolution

STATE OF MECHANICAL MODELLING IN 2016

- **Formulations were available and incorporated in THM-tools**
  - Several approaches and codes
  - Limited testing
- **Applied in earlier EC projects**
  - E.g. PEBS (Long-term performance of engineered barrier systems)
- **Tested in international model verification projects**
  - E.g. Decovalex and EBS Task Force
- **Included in some safety cases**
- **However:**
  - Limited scope
  - Limited number of teams
  - Limited documentation

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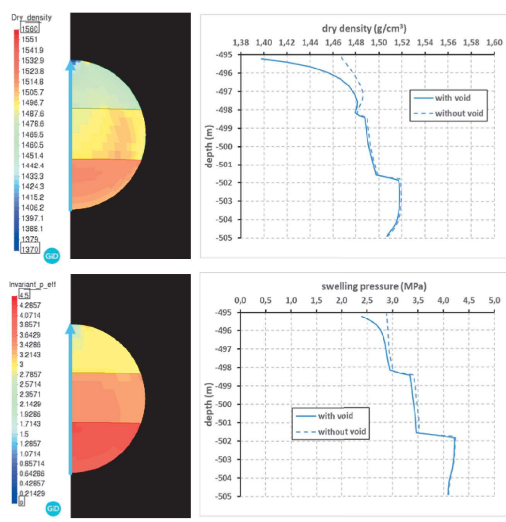
BEACON
Bentonite Mechanical Evolution

STATE OF MECHANICAL MODELLING IN 2022

- **10+ teams are able to model the mechanical evolution of a bentonite barrier!**
- A number of formulations with different strengths and weaknesses have been used
- The experimental work has increased the understanding about which phenomena are important
- Available relevant experimental information has been collected and documented in a database
- Information about available codes has been documented
- The BEACON project has increased the awareness and the competence around the mechanical evolution of bentonite barriers
  - In both advanced and early stage programs



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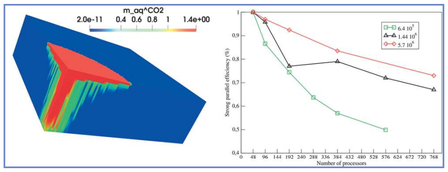
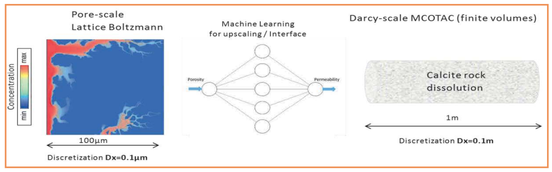
DONUT: DEVELOPMENT AND IMPROVEMENT OF NUMERICAL METHODS AND TOOLS FOR MODELLING COUPLED PROCESSES

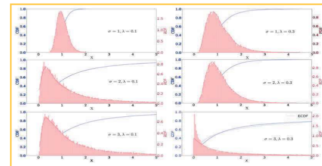
Task 1 Management



Task 2 Numerical methods for high performance computing of coupled processes



Task 3 Scale transition schemes for coupled processes



Task 4 Tools and methods to quantify/derive uncertainties induce by coupled processes

Task 5 Benchmarks of methods and tools for coupled processes

BENCHMARK OF METHODS AND TOOLS FOR COUPLED PROCESSES

- In addition to the specific work that will be conducted by each partners, a specific outcome of DONUT is the definition of benchmarks **that will be use both inside DONUT and outside to foster interactions.** While international benchmarks initiative are existing (Steefel et al., 2015; Birkholzer et al., 2019; Bildstein et al., 2021), the goal here is to define benchmarks of methods and tools to quantify efficiency and added-value in terms of :
  - increase of knowledge (e.g. better physical representation, integration of couple processes),
  - accuracy, robustness, computational cost,
  - robustness of scale-transition approaches,
  - ability to manage uncertainty and sensitivity analyses

Siam initiative https://meetings.siam.org/sess/dsp_talk.cfm?p=111450.

Machine Learning and Geochemistry → ACED & FUTURE WPs; PREDIS

THM model evaluation → HITEC

Multiphase multicomponent reactive transport → ACED & GAS WPs; ↑ Siam initiative

FOCUS ON THE MACHINE LEARNING AND GEOCHEMISTRY BENCHMARK

- **This benchmark aims in providing a point of reference for testing and addressing the challenges relevant to:**
  - Producing high quality training datasets, which will be possible to be used by all available ML techniques.
  - Using Deep neural network learning, Polynomial Chaos Expansion and Gaussian processes to learn from the generated data
  - Testing the accuracy of predictions for geochemical calculations, reactive transport and uncertainty analysis.

MACHINE LEARNING AND GEOCHEMISTRY BENCHMARK: SO FAR > 10 MODELLING TEAMS

- CROSS-EURAD Collaborative effort
- Participants inside/outside EURAD continue to join
- Meetings every 1-2 months to discuss progress
- Joint Development of methodologies and codes. Modelling teams are working closely together.
- Open source software is heavily used. Progress may be followed at anytime at project place: https://service.projectplace.com/#project/1773878474/documents/1964331616

#CLAY00634

GEOCHEMISTRY AND MACHINE LEARNING BENCHMARK WITHIN EURAD

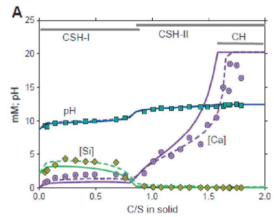
TOPIC 08: Fluid flow and radionuclide migration

N. Prasianakis [1], E. Laloy [2], D. Diederik [2], H. Meeussen [3], C.H. Tournassat [4], G.D. Miron [1], D.A. Kulik [1], M. Marques [1], S.V. Churakov [1, 5], P. Sochala [6], V. Montoya [7], J. Samper [8], O. Kolditz [7], F. Claret [6].
[1]Laboratory For Waste Management, Paul Scherrer Institut - Villigen (Switzerland), [2]Engineered And Geosystems Analysis, Belgian Nuclear Research Centre - Mol (Belgium), [3]Nuclear Research And Consultancy Group (nrg) - Petten (Netherlands), [4]Institut Des Sciences De La Terre D'orléans, Université D'orléans—cnrs/insu—brgm - Orléans (France), [5]Institute for Geological Sciences, Bern University - Bern (Switzerland), [6]Brgm - Orléans (France), [7]Department Of Environmental Informatics, Helmholtz Centre For Environmental Research, Ufz - Leipzig (Germany), [8]Universidade Da Coruña, Centro De Investigaciones Científicas, Enresa, Universidade Da Coruña - A Coruna (Spain)

ML AND GEOCHEMISTRY BENCHMARK: TWO RADWASTE RELEVANT SYSTEMS

- **Two systems of Interest: cementitious system and Uranium sorption system**
  Generation **of training dataset** using PHREEQC, GEMS, ORCHESTRA geochemical solvers
  (Already verified that all three solvers give very accurate and consistent results).
- **Cementitious system**
  Systems of increased complexity are considered: Solutions of $CaO\text{-}SiO_2\text{-}H_2O$ and their equilibration is considered, with the precipitation of CSH-phases and by considering solid solutions. At the next level CO_2 will be considered
- **Uranium system**
  Uranium Sorption on Montmorillonite is considered
  Solutions of Ca-U(VI)-NaCl and their equilibration/sorption including surface complexations is considered. At the next level CO_2 and $CaCl_2$ in solution will be considered

Toward integration in RTM



Modified from D. Kulik CCR 41 (2011) 477–495

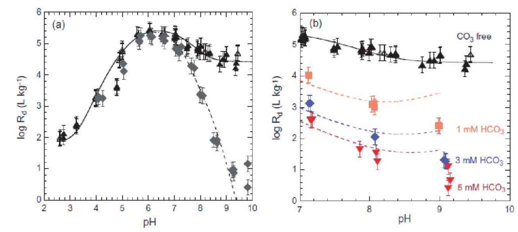


Fig. 3. U(VI) sorption edge measurements on Na-SWy-1 in the absence of carbonate (▲, △) and (a) in equilibrium with atmospheric pCO_2 (◆); (b) in the presence of 1, 3 and 5 mM $NaHCO_3$. Dashed lines: modelled curves with modified stability constants for aqueous U(VI) carbonate complexes.

Modified from M. Marques Fernandes et al. GCA. 93 (2012) 262–277

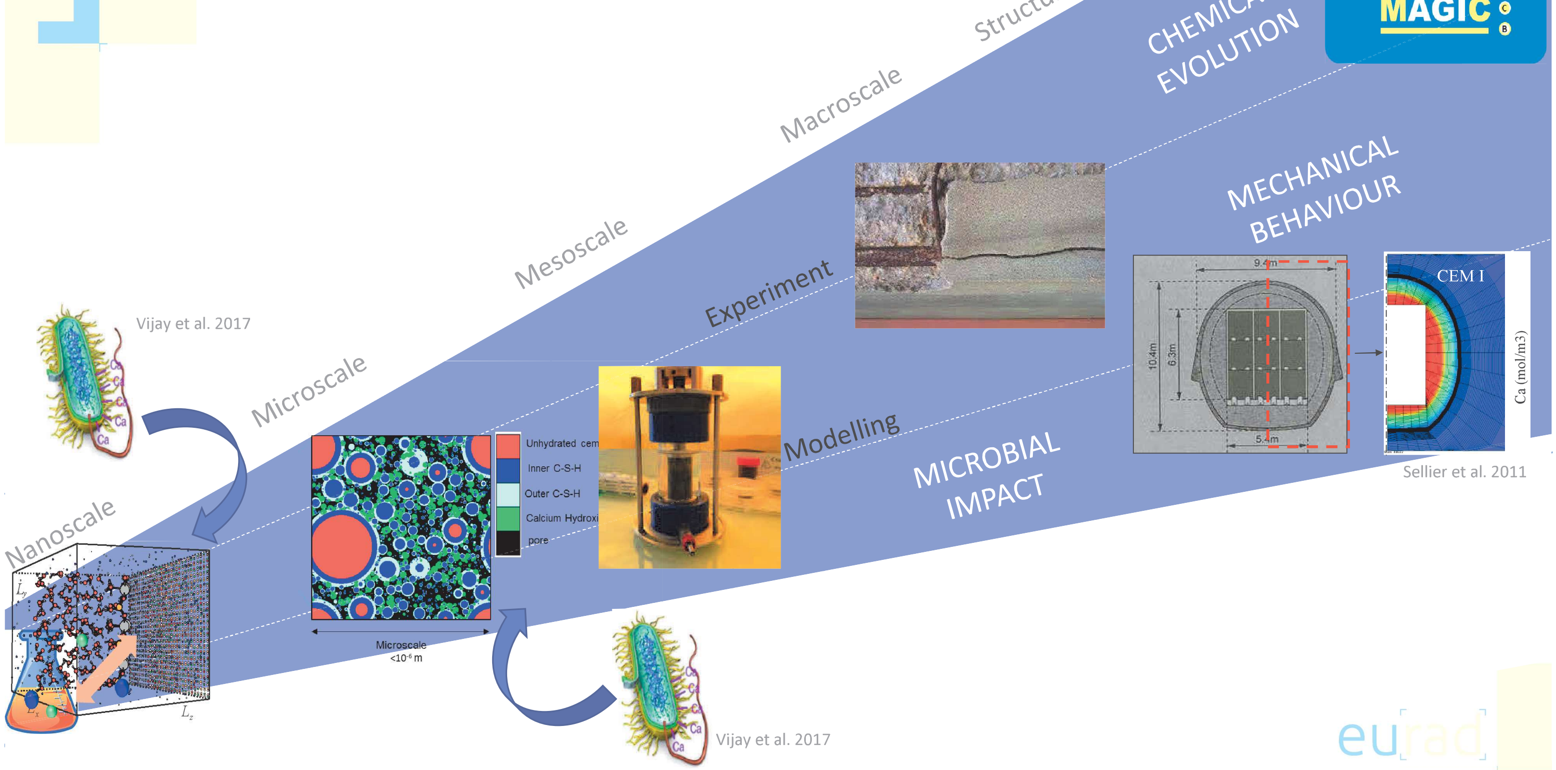
MAGIC : CHEMO-MECHANICAL AGING OF CEMENTITIOUS MATERIALS

OBJ1 - To quantify the chemo-mechanical multi-scale evolution of cementitious materials under the chemical degradation expected in repository environments. To identify the main reactive pathways at the repository scale during the re-saturation phase and at the saturated conditions.

OBJ2 - To obtain a reference chemo-mechanical model of Portland and low-pH concretes exposed to relevant disposal environments, considering representative boundary conditions.

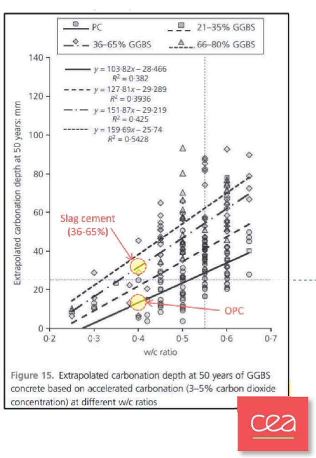
OBJ3 - To estimate the extent of the impact of microbial activity on concrete properties (low-pH and Portland cement) in partially and fully saturated media.

THE MAGIC WP PHILOSOPHY

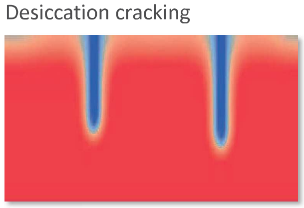


MODELLING AT DIFFERENT SCALES

Continue scale models



Desiccation cracking



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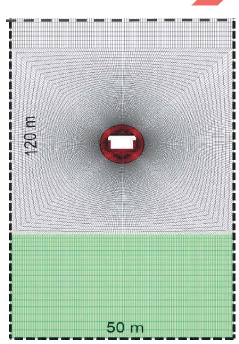
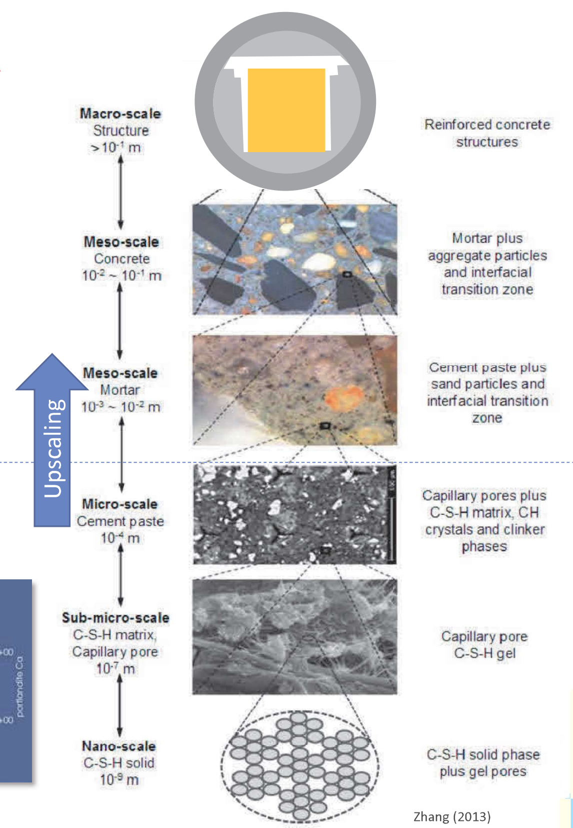
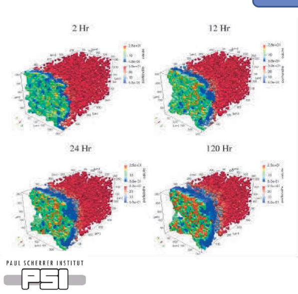
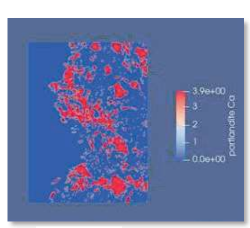




Pore scale models





sck cen

Cracking
→ Major concern in waste management

FROM INDIVIDUAL CONTRIBUTION TO COMPLEMENTARY ADDED VALUE

"Individual efforts can bring excellence but only collective efforts can deliver effectively." Narendra Modi

FROM INDIVIDUAL CONTRIBUTION TO COMPLEMENTARY ADDED VALUE

- Every project by itself will bring novelty and scientific excellence by answering the research questions defined in the project, will integrate knowledge from different scientific communities (geologist, geochemist, physicist, geomechanician, mathematician, enginieers…)
- They complement each other with the final goal to have a holistic understanding and description of the evolution and performance of the EBS leading to a scientific basis for integrated multiphysic-multiscale modelling of that system, bringing an even bigger added value.

SCIENTIFIC DISSEMINATION

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ScienceDirect
Comput. Methods Appl. Mech. Engrg. 369 (2020) 113210
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

On crack opening computation in variational phase-field models for fracture

Keita Yoshioka[a,*], Dmitri Naumov[a,b], Olaf Kolditz[a,c]

Environmental Modelling and Software 145 (2021) 105199
Contents lists available at ScienceDirect
Environmental Modelling and Software
journal homepage: www.elsevier.com/locate/envsoft

porousMedia4Foam: Multi-scale open-source platform for hydro-geochemical simulations with OpenFOAM®

Cyprien Soulaine[a,*], Saideep Pavuluri[a,b], Francis Claret[b], Christophe Tournassat[a,c]

[a] Institut des Sciences de la Terre d'Orléans, CNRS, Université d'Orléans, BRGM, Orléans, France
[b] BRGM, French Geological Survey, Orléans, France
[c] Energy Geosciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

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Geochimica et Cosmochimica Acta 291 (2020) 126–143
Geochimica et Cosmochimica Acta
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Neural network based process coupling and parameter upscaling in reactive transport simulations

Nikolaos I. Prasianakis[a,*], Robin Haller[a,b], Mohamed Mahrous[a,b], Jenna Poonoosamy[c], Wilfried Pfingsten[a], Sergey V. Churakov[a,b]

[a] Laboratory for Waste Management, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
[b] University of Bern, Institute of Geological Sciences, CH-3012 Bern, Switzerland
[c] Institute of Energy and Climate Research (IEK-6): Nuclear Waste Management and Reactor Safety, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

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Mathematics and Computers in Simulation 189 (2021) 55–68
MATHEMATICS AND COMPUTERS IN SIMULATION
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Original articles

Parameter identification for heterogeneous materials by optimal control approach with flux cost functionals

Jaroslav Haslinger[a,1], Radim Blaheta[a,1,2], Raino A.E. Mäkinen[b,*]

[a] Institute of Geonics of the Czech Academy of Sciences, Studentská 1768, 708 00 Ostrava-Poruba, Czech Republic
[b] Faculty of Information Technology, University of Jyvaskyla, P.O. Box 35, 40014 Jyvaskyla, Finland

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Available online 13 June 2020

- Many publications & disseminations actions (e.g. conference)
- Wide journals scope
- Those publications improve our multi-physical understanding of EBS and foster cross fertilisation

A CONTRIBUTION TO KNOWLEDGE MANAGEMENT

Technical Report Full-text available

State Of the Art Report in the fields of numerical analysis and scientific computing

February 2021

Report number: Deliverable n. 4.1

Etienne Ahusborde · B. Amaziane · Baksay A. · Show all 47 authors · Diederik Jacques

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