



ACED/DONUT

EURAD ACED – DONUT Final Workshop

**WORKSHOP - Assessing the long-term evolution of engineered barrier systems of waste disposal systems**

*Date: 2023-11-08 – 2023-11-10*

*Place: Lamot Mechelen – Congress and heritage center, Mechelen, Belgium*

## Program overview (preliminary)

Wednesday 8 November 2023

08u30		Registration
08u45-09u00		Welcome
09u00-09u25	<u>D. Jacques</u> (SCK CEN)	ACED
09u25-09:50	<u>F. Claret</u> (BRGM)	DONUT
<b>Large-scale modelling</b>		
9u50-10u15	<u>J.C.L. Meeussen</u> (NRG)	Development and evaluation of a fast geochemical solver module for coupling with THMC models
10u15-10u40	<u>T. Lamminmäki</u> (Posiva), O. Silva (Amphos21), A. Palacios (Amphos21), A. Iraola (Amphos21), L. Koskinen (Posiva), A. Nardi (Amphos21), G. Roman-Ross (Amphos21), A. Sainz (Amphos21), P. Pitkänen (Posiva), O. Riba (Amphos21), T. Karvonen (Waterhope), J. Molinero (Amphos21)	OLkiluoto State-of-Art Reactive hydrogeochemical modelling, OL-STAR
10u40-11u10	Coffee Break	
11u10-11u35	<u>M. Hokr</u> (TUL), J. Sembera (TUL), J. Stoullil (University Chemistry and Technology Prague), L. Baborova	Double-case canister lifetime evaluation with reactive-transport and chemo-mechanical models

	(CTU), E. Bedrnikova (UJV Rez), P. Vecernik (UJV Rev), D. Vopalka (CTU), M. Hasal (Institute of Geonics), J. Novak (TUL), Z. Michalec (Institute of Geonics)	
11u35-12u00	<u>A. Idiart</u> (Amphos21), A. Sainz Garcia (Amphos21), M. Laviña (Amphos21), E. Coene (Amphos21), C. Plua (Andra), M.-N. Vu (Andra), M. Souley (Ecole des Mines)	Multi-phase flow and geomechanics modelling of gas injection in Comsol Multiphysics
12u00-12u25	T. You (UFZ), M. Mollaali (UFZ), O. Kolditz (UFZ), T. Cajuhi (Federal Institute for Geosciences and Natural Resources) K. Yoshioka (Montanuniversität Leoben)	Hydro-mechanical modeling of crack propagation
12u25-13u45	Lunch Break	
13u45-14u10	<u>J. Oving</u> (NRG), H. Meeussen (NRG), K. Browning (NRG), J. Bartol (COVRA)	Radionuclide solubility in chemical environments occurring in rock salt repositories
14u10-14u35	<u>E. Neeft</u> (COVRA), T. de Bruin (COVRA), R. van Kleef (COVRA), E. Penning (COVRA)	Saturation dependent ingress of reactive gases in geological disposal representative concrete
14u35-15u00	F. Vehling (UFZ), G. Kosakowski (PSI), <u>H. Shao</u> (UFZ)	Two-Phase Reactive Transport Modelling of Heterogeneous Gas Production in Low- and Intermediate-level Radioactive Waste Repository
15u00-15u25	<u>D. Jacques</u> (SCK CEN), S. Liu (SCK CEN), J. Govaerts (SCK CEN)	Modelling waste-packages and cell disposal scale with a generic coupled reactive transport model.
15u25-15u55	Coffee Break	

15u55-16u20	J. Samper (UDC), <u>A. Mon</u> (UDC), L. Montenegro (UDC)	Reactive transport models of the interactions of corrosion products, glass dissolution and bentonite in a HLW repository in granite
16u20-16u45	<u>L. De Windt</u> (Mines Paris), E. Veilly (IRSN)	Chemical evolution of the full glass/steel/cement/claystone system in a HLW disposal cell
<b>Abstraction – Uncertainty – Sensitivity</b>		
16u45-17u10	<u>G. Kosakowski</u> (PSI)	Waste Package Modelling with a Mixing Tank Approach
17u10-17u35	<u>D. Grigaliuniene</u> (LEI), P. Balcius (LEI), P. Poskas (LEI)	Evolution of parameters in intermediate level waste disposal cell constructed in a deep geological repository in granitic host rock: abstracted model results
17u35-18u00	<u>Y. Gu</u> (VTT)	Assessment of chemical evolution at the ILWdisposal cell scale surrounded by granitic host rock by 1-D abstracted model

## Thursday 9 November 2023

08u45-09u10	<u>I. Dimov</u> (IICT-BAS), R. Georgieva (IICT-BAS), I. Ivanov (TUS)	Advanced Stochastic Algorithms for Uncertainty Analysis
09u10-09u35	<u>J. Samper</u> (UDC), C. Lopez (Univresidad Ort), A. Mon (UDC), B. Pisani (UDC), A. Samper (UDC), J. Samper II (UDC), F. Lentijo (ENRESA)	Global sensitivities for reactive transport simulations in a HLW repository in granite
09u35-10u00	<u>P. Socholla</u> (CEA), C. Chiaberge (BRGM), F. Claret (BRGM), C. Tournassat (ISTO, Université d'Orléans)	Dimension reduction for uncertainty propagation and global sensitivity analyses of a cesium adsorption model

10u00-10u25	F. Jankovsky (UJV), M. Zuna (UJV), S. Pospiech (HZDR), V. Brendler (HZDR), U. Noseck (GRS), A. Schneider (GRS), D.-A. Becker (GRS)	Block experiment as an application case for characterization and quantification of uncertainties in RN migration in crystalline formations
10u25-10u55	Coffee break	
<b>Study on phenomena at interfaces – Experimental and modelling studies</b>		
10u55-11u20	J. Goethals (Subatech), <u>C. Wittebroodt</u> (IRSN), L. De Windt (Mines Paris), B. Zajec (ZAG), V. Detilleux (BEL V)	Interaction between carbon steel and cementitious materials in anoxic conditions: effects of imperfect interface and temperature (80°C)
11u20-11u55	<u>P. Wersin</u> (UBern), M. Kiczka (UBern), J. Hadi (UBern), A. Jenni (UBern), J. Goethals (Subatech), J.-M. Grenéche (Le Mans Université), O.X. Leupin (Nagra), N. Diomidis (Nagra)	Iron-Bentonite Interactions in HLW Disposal Cells: Key processes and selected findings from ACED WP2
11u55-12u20	<u>M. Fabian</u> (CER), O. Czompoly (CER), I. Tolnai (CER), L. De Windt (Mines Paris)	Interactions between C-steel and blended cement in concrete under radwaste repository conditions at 80 °C
12u20-13u50	Lunch Break	
13u50-14u15	A. Delanoe	
14u15-14u40	<u>M. Kiczka</u> (UBern), J. Hadi (UBern), A. Jenni (UBern), P. Wersin (UBern), J. Goethals (Subatech), J.-M. Grenéche (Le Mans Université), O.X. Leupin (Nagra), N. Diomidis (Nagra)	Iron(II)-montmorillonite interaction: experimental results and modelling for dispersed and compacted systems

14u40-15u05	J. Samper (UDC), <u>A. Mon</u> (UDC), L. Montenegro (UDC)	Reactive transport models of the interactions of corrosion products and unsaturated FEBEX bentonite of laboratory test and FEBEX in situ test
15u05-15u30	<u>M. Deburé</u> (BRGM)	Insight of the reactive transport models developed to understand the corrosion processes of high-level nuclear waste
15u30-16u00	Coffee break	
16u00-16u25	S. Liu (SCK CEN), K. Ferrand (SCK CEN), J. Goethals (Subatech), D. Jacques (SCK CEN), K. Lemmens (SCK CEN)	Reactive transport modelling of mockup tests to investigate the interaction between HLW glass and ordinary Portland cement
16u25-16u50	<u>Y. Yang</u> (FZJ), R. Patel (KIT), N. Prasianakis (PSI), S. Churakov (PSI), J. Poonoosamy (FZJ), D. Bosbach (FZJ)	Pore-scale Modelling of Solute Transport in Partially and Fully Saturated Porous Media
<b>Benchmarks</b>		
16u50-17u15	I. Dimov (IICT-BAS), <u>R. Georgieva</u> (IICT-BAS), I. Ivanov (TUS)	Case Studies Benchmark at Large-scale Sensitivity Analysis Studies
17u15-17u40	<u>J. Samper</u> (UDC), A. Mon (UDC), L. Montenegro (UDC), B. Amaziana (E2S UPPA), E. Ahusborde (E2S UPPA), T. Xu (Jilin University), Y. Han (Jilin University), Y. Yuan (Jilin University), J. Sembera (TUL), M. Hokr (TUL), A. Narkuniena (LEI), G. Poskas (LEI)	Benchmark case for non-isothermal multiphase flow and reactive transport for radioactive waste disposal
19u00-	Dinner	

## Friday 10 November 2023

Machine Learning in Reactive Transport Modelling		
08u50-09u25	<u>N. Prasianikis</u> (PSI), E. Laloy (SCK CEN), D. Jacques (SCK CEN), J.C.L. Meeussen (NRG), C. Tournassat (UOrléans), G.D. Miron (PSI), D.A. Kulik (PSI), A. Idiart (Amphos21), E. Demirer (Amphos21), E. Coene (Amphos21), B. Cochevin (Andra), M. Leconte (Andra), M. Savino (Andra, UParis-Saclay), J. Samper II (UDC), M. De Lucia (Helmholtz Centre Potsdam), S.V. Churakov (PSI, UBern), O. Kolditz (UFZ), C. Yang (Environmental Data Technology), J. Samper (UDC), F. Claret (BRGM)	Overview of the geochemistry and machine learning benchmark within EURAD Joint Project
09u25-09u50	<u>J. De Sanctis</u> (Sogin S.p.A.), F. Marconi (Sogin S.p.A), M. Rosati (Sogin, S.p.A.)	Sensitivity analysis of the main radionuclide transport parameters through the EBS of a Near Surface Nuclear Waste Repository by means of machine learning techniques
09u50-10u15	<u>E. Laloy</u> (SCK CEN), J. Govaerts (SCK CEN), D. Jacques (SCK CEN)	Speeding up reactive transport simulation in cement systems by surrogate geochemical modelling: how to obtain a sufficiently representative training set
10u15-10u45	Coffee Break	
10u45-11u15	<u>E. Desmirer</u> (Amphos21), E. Coene (Amphos21), A. Iraola (Amphos21), A. Idiart (Amphos21)	Surrogate models for geochemical simulation of cement degradation based on Artificial Neural Networks

11u15-11u40	<u>M. De Lucia</u> (GFZ), M. Kühn (GFZ, UPotsdam), M. Lübke (UPotsdam), B. Schnor (UPotsdam)	Combining approximated computing and hardware accelerators in coupled reactive transport simulations: POET
11u40-12u05	J. Samper Jr (UDC), <u>J. Samper</u> (UDC), C. Yang (Environmental Data Techniques), A. Mon (UDC), F. Lentijo (ENREDA)	Contribution of UDC/ENRESA to the Machine Learning Geochemical benchmark with Gaussian Processes and random forests
12u05-12u30	N.N.	A glance to the future – digitization and digital twins in long-term management of radioactive waste
12u30-12u40	<u>F. Claret</u> (BRGM), <u>D. Jacques</u> (SCK CEN)	Closure