Cement-based materials, properties, evolution, barrier functions

Newsletter Issue 2, November 2016

Foreword

Cebama is a research and innovation action granted by the European Atomic Energy Community in support of the implementation of the first-of-the-kind geological repositories. The 4-year project, started 1st of June 2015, is carried out by a consortium of 27 partners consisting of large Research Institutions, Universities, one TSO, and one SME (small medium enterprise) from 9 EURATOM Signatory States, Switzerland and Japan. National Waste Management Organizations support Cebama by co-developing the work plan, participating in the End-User Group, granting co-funding to some beneficiaries, and providing for knowledge and information transfer.

The overall strategic objective of Cebama is to support the implementation of geological disposal by significantly improving the knowledge base for the Safety Case for European repository concepts. Scientific/technical research in Cebama is largely independent of specific disposal concepts and addresses different types of host rocks, as well as bentonite. Cebama is not focusing on one specific cementitious material, but is studying a variety of important cement-based materials in order to provide insight on general processes and phenomena which can then be transferred to several different applications.

This is the second newsletter of the project and gives a briefing of the results and the advance of the working programme presented at the first annual workshop, held in Barcelona in May 2016. Details on the structure and formal issues of the project can be found in our website www.cebama.eu.

Enjoy it!

Marcus Altmaier (Cebama Coordinator)

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Editorial

Dear Reader,

We have the pleasure to present the second issue of the newsletter of the Horizon 2020 project Cebama which started on June 1st 2015.

The main purpose of this newsletter is to inform a wide interested community on the research carried out within Cebama during its running period. An overview of the ongoing activities and recent achievements of the project can be found in the following pages.

The first Annual Workshop was held in Barcelona, in May 2016, which represented an important milestone in the working programme. The proceedings of the workshop are ready to download from our webpage, have a look at www.cebama.eu.

Amphos 21

Knowledge management and dissemination office of Cebama

The consortium

27 beneficiaries consisting of Research Institutes, Universities and SMEs from 9 EU members countries, Switzerland and Japan contribute to Cebama

9 End User Waste Management Organizations

WP1 Experiments on interface processes and the impact on physical properties

WP leaders : Erika Holt (VTT, Finland), Francis Claret (BRGM, France), Urs Mäder (University of Bern, Switzerland)

The 1st workshop provided the third extensive discussion group for workpackage 1, after our earlier focused WP1 meeting which took place in London (November 2015) and the project kick-off meeting (Brussels, July 2015). Some partners had multiple persons attending, including participation of new junior staff or students getting integrated to the project and waste management topics. During the WP1 plenary session, there were scientific progress updates provided by 17 partners during the 3 hour session. The previous day at the workshop, during WP1 detailed discussions, progress was reviewed regarding aspects such as cooperative benchmark studies, exchange of samples and synergy between experimental methods. There were also inputs from the End Users group regarding the applicability of methods and selected materials. The topical session on lessons learned from other projects on cementitious barriers also provided complimentary information to be linked with CEBAMA, such as:

- DOPAS project (Marja Vuorio, Posiva) where concrete and bentonite have been used in tunnel end plugs with initial state material design, construction, modelling and performance monitoring
- ECOCLAY-II (Nicolas Michau, ANDRA) explaining compatibilities between clay (granite) and cementitious material and their evolution

A major outcome from earlier discussions at the WP1 meeting in London had been the need for a common baseline concrete material for comparative studies with national recipes. The 1st workshop then shared about the agreed-upon requirements for this mixture, its laboratory production and distribution to partners. A ternary low-pH mixture was produced, using both silica fume and blast furnace slag with a calcium-silica ratio of the binder being 0.61. The produced mixture had workability (slump) of 180 mm, air content of 0.9% and density of 2450 kg/m3, with the appearance as shown in Figure 1. An additional paste reference mixture was also made. Approximately 40 samples were distributed in spring and early summer to 6 different partners, and more sample were available upon request. Other partners have used the benchmark methodologies for preparing local samples, for instance in the Czech Republic (Figure 2). The expectation is that the benchmark low-pH concrete and paste samples will allow for comparable test result interpretation and better cooperative development of methodologies for interpreting material performance that also comes from existing aged samples (i.e. Figure 3). More comprehensive results and first results from the benchmark studies will be available by the second workshop and ready for inputs to WP3 modelling.

At the workshop, WP1 partners gave updates about their resources, schedule and dissemination activities. During the first year, some of the partners have been in the process of hiring students and staff to fulfil the work plans and ensure competence development of the next generation of nuclear waste management experts. Partners have been interacting with end users groups to determine the highest priority for cementitious material recipes and exposure conditions in the experimental studies, which will best serve the quantitative modelling and long-term safety evaluations. Regarding dissemination plans, many WP1 partners participated and presented at the "Mechanisms and Modeling of Waste/Cement Interactions" workshop in Murten, Switzerland on May 22-25, 2016 (see www.empa.ch/cement2016). Some of the partners also shared at the FP7 DOPAS project ending seminar (Turku, Finland on May 25-27, 2016) on "Full-Scale Demonstration of Plugs and Seals", where concrete-bentonite interaction may also be an issue for long-term safety and performance (see http://www.posiva.fi/en/dopas/dopas_2016_seminar). Preparations are underway for participation to the Clay Barriers conference (Switzerland, September 2017) for further dissemination of WP1 achievements (see http://www.clayconferencedavos2017.com/).

The activities of Work-package 1 during the first year of the project have addressed the synergy between various research methods and experimental studies of cementitious materials used in the repositories. At the start of the project an internal survey of WP1 participants was done to gather more details that served as the basis for the deliverable reports of the first year. This has included discussions and information on experimental methods and cementitious materials being studied, to ensure cooperation and implementation by the end users group. The first Deliverable report D1.01 provided detailed scientific work summary plans from each partner, serving as a basis for future reference. The next Deliverables D1.02 on systems to be studied, D1.03 as a state-of-the-art report on WP1 topics to be used as external reference by the general public, D1.04 as Experimental method boundary conditions to be used in WP1 studies, and D1.05 on Experimental materials to be used in the WP1 program were all available by or near the workshop time.

Figure 1. Slump of CEBAMA WP1 benchmark reference concrete, produced at VTT.

Figure 2. Preparation of bentonite suspension, at UJV.

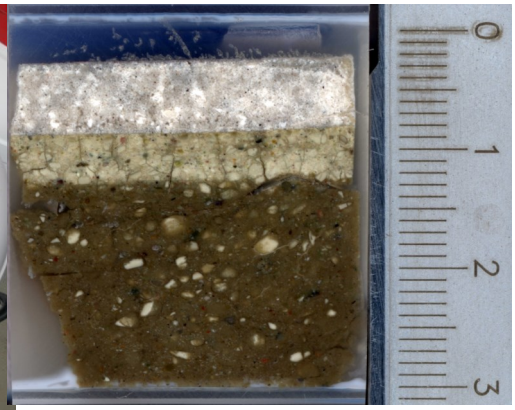

Figure 3. Example of investigation of aged concrete -bentonite interface within a concrete plug in a granite gallery context (study by UAM).

WP2 Radionuclide retention

WP leader : Bernd Grambow (Armines, France)

The objective of WP2 is the study radionuclide retention processes in high pH concrete environments. The work conducted is largely independent of specific disposal concepts and addresses different types of host rocks. The aim is to provide insight on general processes and phenomena and their couplings in overall interaction mechanism, which can then be transferred to different disposal situations and water access scenarios in a high pH repository environment with cementitious materials. It also assesses the impact of chemical alterations (e.g., high pH concrete ageing, carbonation, transition from oxidizing to reducing conditions) on radionuclide retention.

A large number of studies are conducted, including leaching and solubility tests, diffusion tests, sorption experiments and co-precipitation studies. Variables are water composition, redox state and solid/water ratios. Also interaction with gaseous radionuclides (C14) is studied. Most experiments consist in exposing a selected radionuclide to fresh or pre-equilibrated solid/water systems for extended periods of times. Solids are a variety of important high pH cement-based materials: fresh and water aged cement pastes CEM I and CEM V, but as well individual phases such as CSH phases of various Ca/Si ratios, LDH and OH, SO_4, Cl of CO_3 type AFm and Aft phases. Radionuclides which have high priority from the scientific and applied perspective are selected. Some radionuclides are replaced by non-radionuclide isotopes. The corresponding chemical elements of interest are in particular Be, C, Cl, Ca, Se, Mo, I, and Ra. The number of systems to study is large. To allow for compatibility between individual approaches the meeting participants agreed to use as far as possible and feasible similar experimental protocols, boundary conditions or similar solids. Experimental programs are coupled to various modelling approaches, allowing to pave a way how for example to go from individual cement phases to the overall cement pastes.

All partners have started their experimental program and/or the respective development of protocols for preparation of individual cement phases. The following presentations of the various partners at the first CEBAMA workshop in Barcelona include a description of a detailed refinement of the experimental procedures, characterization of solid phases and of protocols for synthesis of cement phases, as well as first results of solubility and retention studies of Be, Ra and Tc on concrete and key cementitious phases

WP3 Interpretation and modelling

WP leader : Andrés Idiart (Amphos 21, Spain)

In recent years, significant advances have been achieved regarding the understanding of coupled physical and chemical processes affecting the performance of cement-based barriers. However, important gaps still exist on the: (1) coupling between chemical changes of cement paste microstructure and its physical properties, (2) relation of classical macroscopic reactive transport models to the microstructural features of cement and concrete, and (3) confidence in extrapolating numerical models of cementitious systems for long-term conditions. The main goal of WP3 is to contribute in filling these gaps by modelling and interpretation of experimental results generated within the project. The focus is mainly on physical and chemical processes that can lead to changes in transport properties both in the cementitious systems as well as their interface with clays or compacted bentonite.

An essential basis for WP3 is the outcome of the experiments and their characterization performed within the project. Every WP3 partner has already established collaborations with WP1 and WP2 to model specific sets of experiments. During the 1st Annual Workshop, new collaborations have been defined and it is expected that more interaction will result from the next Annual Workshops, as more results start becoming available.

Experimental results from the project will in general not be available until much later. Therefore, each WP3 partner is using existing experimental data, relevant to their objectives within the project, in order to test and verify their modelling approaches and main developments during the first stages of the project.

During the 1st Annual Workshop, all WP3 partners from 13 organizations presented their progress, while 8 S&T contributions from WP3 are presented here. Three students from FZJ, UDC and PSI are doing their PhD within WP3. The models under development mainly focus on:

1) cement/concrete matrices and cement/clay interactions,
2) reactive transport models, also coupled to hydro-mechanical models,
3) mostly at the laboratory length scale, but also at pore- and macro-scale,
4) time scales mostly covering the duration of lab tests, but also long-term predictions.

KIT S&T presents the conceptual model to be used in continuum-scale reactive transport simulations of dedicated experiments of the interaction between low pH cement paste and bentonite water. The model will be implemented in iCP, coupling Comsol Multiphysics and Phreeqc. As presented in the workshop, VTT will also model degradation of low-pH cement systems. In turn, NRG will model 1D reactive transport processes at the interface between cement paste and Boom clay, using the open-source framework ORCHESTRA. CTU S&T presents an experimental setup for measuring diffusion coefficients in a sandwiched bentonite cement arrangement and its interpretation through 1D modelling using GoldSim. During the workshop, the research plan to implement a new code for modelling reactive transport processes in cement/clay interfaces was presented by PSI, including electrochemical couplings (Nernst-Planck equations).

BRGM S&T presents their research plan to perform streaming potential and spectral induced polarization experiments to describe the surface electrical, petrophysical, and mineralogical properties of low pH cement pastes. The method to interpret experimental measurements with surface complexation and transport models at the pore and sample scales is described with the final goal of improving the predictions of reactive transport properties.

JUELICH S&T presents their plan and preliminary developments of a new implementation of a pore-scale reactive transport model to study degradation processes in the cementitious matrix. The numerical framework makes use of the existing software Palabos and Phreeqc, and a verification example is shown. During the workshop, SCK·CEN presented their plans about pore-scale reactive transport modelling using their numerical tool YANTRA, which is in a more mature development stage. Different experiments will be interpreted by each partner, giving new insights in reactive transport processes at a more fundamental scale compared to traditional continuum models.

RWMC S&T introduces an application modelling case of the effect of secondary minerals on cement-clay and cement-bentonite interactions under repository conditions. A coupled hydro-chemo-mechanical framework is presented, using the reactive transport code Phreeqc-TRANS and the hydro-mechanical code DACSAR-BA. A different approach for modelling coupled chemo-mechanical processes in concrete is presented by LML in their S&T, based on homogenization theory and advanced nonlinear constitutive models. The model results are compared to experimental data on several degradation processes under laboratory conditions.

In the same line, Amphos 21 S&T describes the chemo-mechanical model implemented in iCP, coupling reactive transport with mechanical and chemical damage models (Figure 4, right). Preliminary results of the simulation of existing experiments at Chalmers University are presented. In turn, UDC S&T focuses on reactive transport processes of concrete-bentonite interaction experiments under non-isothermal conditions. The model takes into account the thermo-hydro-chemical couplings and their impact on mechanical behaviour using the code INVERSE-FADES-CORE developed at UDC. Preliminary results of the model applied to the interaction of OPC concrete and FEBEX bentonite are presented.

Finally, ANDRA presented their plan to model reactive transport processes in low-pH concrete components at the macro-scale and their interface with clayey systems. They will integrate data acquired within CEBAMA to conduct long-term Performance Assessment models at a larger spatial scale.

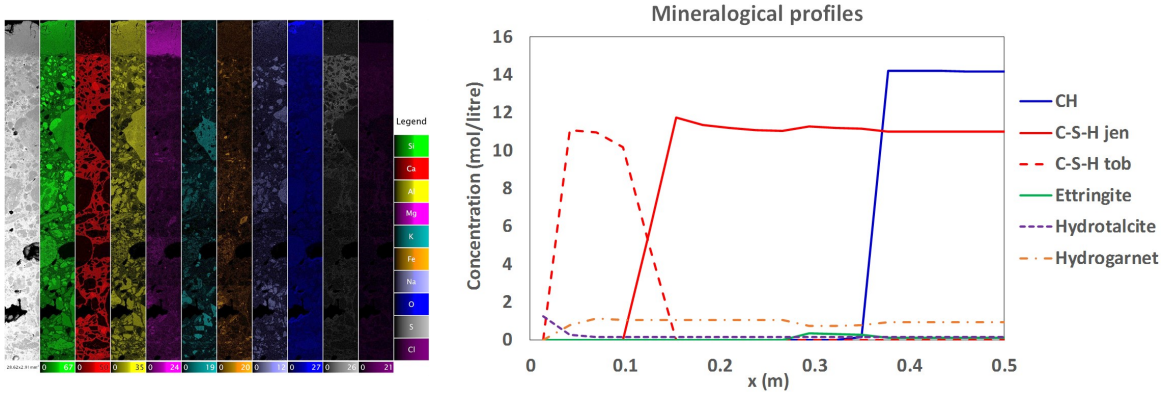

Figure 4: Left: Example of chemical mapping by SEM-EDX (work of UAM); right: 1D profile of mineralogical composition of concrete after 10 000 years of calcium leaching (from left to right) (Amphos 21)

Events

First Annual Workshop (May 11th to 13th 2016, Barcelona)

The 1st Annual Workshop was held in Barcelona (Spain), 11-13 May, 2016. The workshop was hosted by Amphos 21. There were 58 attendees at the workshop, representing beneficiaries, the End-User-Group and project external organizations.

The workshop was organized in three days of oral presentations describing the work performed by the beneficiaries, a topical session on "Lessons learned from previous and current projects on cementitious barriers" and individual WP session focused on enhance the interaction between the partners and between WP.

An electronic copy of the proceedings of the 1st Annual Workshop of CEBAMA is available at the project website (www.cebama.eu)

Next events

The project's **Second Annual Workshop** will take place in Helsinki (Finland) and hosted by VTT. The approximate date of the 3-days workshop is the week of 15-19 May 2017.

The workshop will be organized in order to each beneficiary has the opportunity of presenting their results. The individual WP sessions as well as the topical session, the poster session and the ExCom/ EUG meetings will also take place.

More information on the workshop venue will be soon available at the Cebama website (www.cebama.eu).