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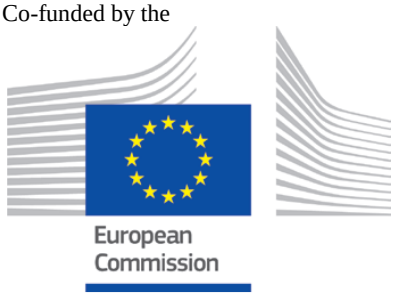

CEBAMA

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List of mobility measures and summary of the works undertaken

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RE	Restricted to a group specified by the partners of the CEBAMA project	
CO	Confidential, only for partners of the CEBAMA project	

ABSTRACT:

The deliverable summarizes the mobility measures organized and funded within Cebama and the work done during these stays.

RESPONSIBLE:

Amphos 21

Five young researchers were granted mobility measures offered by the Cebama project. The grant covered their stays (e.g. accommodation, daily allowance, transport, etc.) with a budget up to 2,000 € per mobility measure. Table 1 provides the list of the assigned mobility measures. The researcher, the sending and hosting organizations, and the Project WP framing the studies are indicated.

Table 1: *List of researchers awarded with mobility measures in Cebama*

Applicant researcher	Sending organization	Hosting organization	WP
Janna Kittnerová	CTU	JUELICH	WP2
Aku Itälä	VTT	AMPHOS 21	WP3
Stephan Rohmen	JUELICH	PSI	WP3
Enrique Rodríguez Cañas	UAM	BRGM	WP1
Marta López García	AMPHOS 21	JUELICH	WP2

A brief summary of the work done during each mobility measure is given below:

Jana Kittnerová (CVUT / JUELICH)

Jana Kittnerova, PhD student at the Czech Technical University (CTU) in Prague, Czech Republic spent 3 months at the Forschungszentrum Jülich (JUELICH) in Germany (January 13, 2018 to April 15, 2018). Her CEBAMA Mobility Measure was framed in CEBAMA WP2, radionuclide retention by high-pH concrete. This internship was part of her PhD studies at the Faculty of Nuclear Sciences and Physical Engineering at CTU. Her work is focused on the interaction of cementitious materials with radionuclides, in particular radioisotopes of radium and strontium, and is led by Barbora Drtinová and Dušan Vopálka. Jana's internship at Forschungszentrum Jülich was hosted by Guido Deissmann and Steve Lange followed by previous work on the sorption of the isotopes ^{223}Ra or ^{85}Sr on real mortar and concrete under conditions relevant to radioactive waste disposal in the Czech Republic. In Jülich, Jana became familiar with the synthesis, preparation and characterization (e.g. SEM, XRD) of calcium silicate hydrate (CSH) phases, the major hydration phases in cementitious materials, which she then used for experiments to get further insight into the uptake mechanisms of ^{226}Ra, ^{133}Ba and ^{90}Sr in cementitious barriers. Besides these experiments the student also dealt with the influence of carbonation on various cementitious materials and its consequences on the sorption properties for ^{226}Ra. In the future, she were establishing the work with CSH - as experienced in Jülich - at CTU, comparing also the results of sorption experiments with ^{226}Ra and ^{223}Ra (which is used as analogue of ^{226}Ra at CTU). The outcome of this visit will provide for additional understanding of the behaviour of safety-relevant radionuclides in cementitious materials in deep geological repositories for radioactive waste.

Marta López García (AMPHOS 21 / JUELICH)

In May/June 2018, Marta Lopéz-García, postdoctoral researcher at AMPHOS21, Barcelona, Spain, spent 2 month as guest scientist at Forschungszentrum Jülich (JUELICH), Germany, in the frame of a CEBAMA Mobility Measure, related to her work within CEBAMA WP2, radionuclide retention by high-pH concrete. The main goal of this mobility measure was to study the adsorption of Mo (as

molybdate) onto specific aluminate phases representative for hydration products in cementitious materials, namely AFm and AFt and mixtures thereof, containing different anions (i.e. carbonate and sulfate). The solid phases synthesized in her home lab in Spain were characterized in JUELICH by various spectroscopic and microscopic techniques including XRD, SEM-EDX, FTIR, and RAMAN as well as by TG-DSC. The uptake kinetics of molybdate by the various AFm/AFt mixtures were investigated in specifically designed batch sorption experiments using equilibrated solid/liquid mixtures for up to 16 days under anoxic and CO_2 free conditions in a glove box (Ar 99.99%). A first analysis of the data indicates a marked difference regarding the Mo retention behavior of the different phases. In the case of samples composed mainly by AFm, Mo retention was found to be extremely effective and fast, whereas at higher AFt percentages, Mo seems only to be poorly retained. The outcome of this visit will provide for additional insights into the migration and retention behavior of Mo in cementitious barriers in repositories for nuclear wastes.

Enrique Rodríguez Cañas (UAM / BRGM)

The mobility measure UAM to BRGM intended to derive microstructural and mineralogical aspects using the methodologies developed by S. Gaboreau and the BRGM team studying both clay and concrete materials. One unaltered block of FEBEX bentonite/concrete was supplied by the Uni-Bern team, with the knowledge of CIEMAT (M.J. Turrero) and Nagra (F. Kober). The sample was impregnated in ^{14}C MMA during more than 4 months in order to achieve full access even to the smectite interlayer porosity. Then, quantitative porosity measurements were done by autoradiography. It became evident, that there is a porosity increase in concrete affecting more than 2 cm thickness from the bentonite contact. This is presumably related to the initial quality of the shotcreting. Dr. Enrique Rodríguez-Cañas (UAM) supervised by S. Gaboreau and J. Cuevas (UAM) was following at BRGM the adquisition of quantitative X-ray intensity maps and BSE images with a Cameca SX Five EPMA microscope equipped with five wavelength dispersive spectrometer (WDS). This allowed to take 512 x 512 pixel elemental maps with a spatial resolution of 2 µm per pixel. It was possible to compute mineral/phase maps based on procedures of chemical segmentation using ternary scatter plot projections. Actually, complete mineralogical maps were processes in order to detect the mineralogical evolution at the microscale related to the geochemical perturbation of the complex mineralogy at the bentonite-concrete.

Aku Itälä (VTT / AMPHOS 21)

PhD student and research scientist Aku Itälä of VTT visited Amphos 21 in Barcelona, Spain, during the period of 12-16.2.2018 for cooperation with CEBAMA WP3 on modelling issues. The host was Andrés Idiart from Amphos 21 who is also the WP3 leader. On this trip Itälä presented AMPHOS some of the CEBAMA WP1 experimental results by VTT as well the CSH model developed at VTT for CSH dissolution. The model was further tested together with Andres Idiart and the complexity of the model was also simplified. Also some comparison between PHREEQC and GEM-Selektor was done.
There was discussion related to the modelling of the VTT experiments and hydration of reference cements. VTT's CSH model was also applied to the hydration model of AMPHOS and tested the workability of the model. There was discussion about the usability of the model of VTT for low pH values (below 0.8). The role of different ion activity models and use of different databases were also clarified, especially regarding the Thermochimie database. Also there was some discussion about the relevant mineral phases in different time spans and some references were changed related to modelling of cement phases. Further co-operation and the use of VTT's CSH model in different

modelling tasks was suggested. The outcomes of this visit are being utilized to enhance the very long-term pH evolution models for Posiva's safety case on the EBS performance expectations.

Stephan Rohmen (JUELICH / PSI)

PhD student Stephan Rohmen of Forschungszentrum Jülich (JUELICH) spent two weeks at the Paul Scherrer Institute (PSI) in Villigen, Switzerland, between 19.02.2018 and 02.03.2018 within the frame of the mobility measures of the CEBAMA project, related to CEBAMA WP3, Interpretation & modelling. His PhD studies, co-supervised by Andrés Idiart from AMPHOS 21 and Guido Deissmann from JUELICH are focused on the development and application of a pore-scale model for the simulation of degradation processes occurring in cementitious materials (e.g. calcium leaching), to get further insights into the effects of chemical and mineralogical changes in cementitious barrier materials on its transport properties. During his stay at PSI he had the possibility to extend collaborations with other groups contributing to WP3 and exchange experiences with other researchers in the domain of pore-scale reactive transport modelling. Discussions with experts in pore-scale reactive transport modelling helped to improve the Lattice-Boltzmann based reactive transport code developed within CEBAMA called iPP. These include the usage of input data from cement hydration modelling, the implementation of a multiscale effective medium approach to model the diffusivity of C-S-H phases, or approaches to model C-S-H as ternary or quaternary solid solutions. In addition, a benchmark activity to compare the results of iPP against another reactive transport code (Yantra) was started. Stephan was also able to attend to the 8th International reactive transport PhD workshop & CEBAMA PhD meeting which took place during his stay at PSI. The outcome and the experiences gained during his mobility measure to visit PSI will enhance the capabilities of iPP and allow for application of iPP to simulation of experiments performed within CEBAMA WP1, thus providing for an enhanced understanding of the coupling between chemical alteration processes in cementitious materials and changes in its physical properties.