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# Consolidated plan for Upscaling Modelling Task.

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**ABSTRACT**

Work Package 3 is devoted to the modelling and interpretation of experimental data generated within CEBAMA. Different modelling approaches are used by each partner, with focus on reactive transport processes that can impact the physical properties of cementitious materials and their interface with clayey systems. Therefore, a common modelling task is needed for a better integration of the results and conclusions obtained in WP3. This report gives details of the proposed plan for such a modelling task. The goal of this task is to cluster WP3 activities around a common simulation case and integrate different spatial and temporal upscaling methods that are planned to be used by each partner. The work related with this activity will be undertaken during a period of approximately 2 years, from the 2nd Annual Workshop in May 2017 to June 2019.

**Keywords:** Upscaling, Modelling Task, Clustering Activity

# 1 INTRODUCTION

Work Package 3 on Modelling and Interpretation gathers a total of 13 partners. The focus of the modelling work is mainly on reactive transport processes that can impact the physical properties of cementitious materials and their interface with clayey systems. However, diverse modelling approaches are used by each partner, focusing on different physical and chemical processes at several scales of analysis. A modelling task that aims at integrating the results and conclusions obtained by each partner is thus needed. The goal is to foster synergies between partners and present the outcomes of WP3 in a more consistent way.

This report presents the plan for the Common Modelling Task. First, a brief analysis of the modelling work in WP3 is presented. The proposed plan follows from this analysis.

# 2 OVERVIEW OF MODELLING APPROACHES IN WP3

In this section, an overview of the systems under study in WP3 is given, together with a summary of the processes and scales of analysis.

## 2.1 Cementitious materials

In WP3, approximately 10 partners will consider low-pH cementitious systems, while 8 partners will focus on high-pH cementitious materials (note that some partners will analyse both systems). However, high-pH cementitious materials under study differ significantly and include CEM I, CEM II and CEM III OPC systems.

In WP1, a benchmark low-pH cementitious material has been proposed, referred to as Cebama reference mix. Cement paste and concrete specimens were cast and distributed to interested partners (concrete: BRGM 3, KIT 3, CSIC 8, VTT; cement paste: Sheffield 10, BRGM 3, Juelich 3, KIT 8, CTU/UJV, VTT). It is expected that a relatively large dataset of the characterization of the reference mixes is obtained both for the intact and aged states. In turn, WP2 focus mainly on radionuclide retention in high-pH cementitious systems, although individual cement hydrates are studied as well, such as C-S-H phases of various Ca/Si ratios, LDH and OH, and AFm and Aft phases.

## 2.2 Clayey materials

Even though one of the goals in CEBEMA is to understand interaction processes between cementitious and clayey systems, not all the partners focus on the processes at the interface. Five partners focus on the interaction of cement-based materials with different water compositions, i.e. not explicitly modelling the clay. The rest of teams consider different clayey systems (2 partners will focus on Boom clay, 1 partner on Opalinus clay, 2 partners on Callovo-Oxfordian clay, and 3 partners on different bentonites, including FEBEX, Czech B75, and Kunigel V1).

## 2.3 Processes

Several physical and chemical processes are studied in WP3. The main focus is on the impact of reactive transport processes on the diffusive and advective properties of cementitious systems. Therefore, chemical reactions and solute transport by diffusion are the main processes studied in WP3. However, some partners consider additional coupled processes, such as thermal effects, fluid flow, mechanical behaviour, surface electrostatics, or electrochemical transport.

## 2.4 Scale of analysis and upscaling

Most of the models will be used to analyse experimental data at the decimetre-scale, representative of the size of laboratory samples. However, some partners will analyse processes at a much smaller scale, i.e. pore-scale models, while other partners will consider the macro-scale, representative of repository conditions.

Several models will consider upscaling at several observation levels, i.e. ranging from pore-scale processes to macroscopic behaviour of repository components. These models consider spatial as well as temporal upscaling. In particular, 5 partners will develop models at decimetre-scale to simulate laboratory experiments and will upscale them in time and space to repository conditions. Other partners will focus on the upscaling of pore-scale and micro-scale processes to the decimetre-scale and multi-scale approaches using homogenization to model the impact of microstructural changes on the macroscopic properties.

# 3 DESCRIPTION OF THE COMMON MODELLING TASK

As mentioned above, the objective of the common modelling task is to cluster WP3 work in a common activity. Given the variety of modelling approaches, processes, and scales of analysis under study in WP3, the goal of the benchmark modelling exercise is not to verify numerical codes over a given detailed model setup. It is noted that several partners have previously participated in benchmarking exercises of numerical codes to verify the tools. Therefore, code benchmarking is out of the scope of the modelling task.

Instead, the common modelling task is devoted to the comparison and integration of the results from different modelling approaches to a given studied system. The selected system is the low-pH cement mix referred to as Cebama reference mix, to profit from the characterization performed in WP1. The clay system will not be modelled explicitly. Instead, interaction of low-pH cementitious material with a generic clay porewater will be studied.

First and second data freezing of experimental data are planned for project months 24 and 36, respectively. At these stages, input data for the models will be updated with latest results on the initial characterization of the reference mix and from preliminary experimental results on its interaction with clayey systems and groundwater simulants.

The modelling task consists of several sub tasks, as described in the following subsections.

## 3.1 Modelling of hydration of the reference mixes (cement paste and concrete)

This step is needed to characterize the hardened cement paste and concrete composition after curing and hydration, which serves as input to reactive transport models. The result of this shall include the phase assemblage of the cement hydrates and the porosity distribution (gel and capillary porosity). Comparison will be done between different approaches adopted in WP3 and with experimental data of the characterization of the initial system (porosity, cement hydrates, microstructure).

## 3.2 Comparison of constitutive relations between transport properties and microstructure

The different constitutive relations between transport properties (i.e. diffusion coefficient and permeability) and microstructure (i.e. porosity, pore size distribution, volume fractions of cement hydrates, microcracks, interfacial transition zones, etc.) will be compared. This comparison will include not only the relations proposed and used by each partner, but shall include feedback from experimental data of the reference mix.

## 3.3 Application of modelling approaches to a simulation test case

An application case is proposed to compare the outcomes of different modelling approaches. It consists of the interaction between a concrete slab and a generic clay porewater, as shown schematically in Figure 1. A one-dimensional setup of a concrete slab made of the reference mix will be considered, with a generic dimension of 10 cm. The slab is in contact on one side to a generic clay porewater. The other end of the slab is closed to solute transport. Solute transport is exclusively by diffusion under fully water saturated and isothermal (25 °C) conditions.

The initial composition of the concrete slab follows from the sub task on hydration modelling. The composition of the generic clay porewater will be defined during the 2nd Annual Workshop in Helsinki, May 2017.

The processes that will be modelled are chemical reactions due to water-cement interaction, diffusion (with or without electrochemical coupling), and coupling between changes in microstructure induced by chemical reactions and transport properties. Even though solute transport is exclusively by diffusion, the evolution of both the effective diffusion coefficient and permeability will be obtained as a result of chemical alteration.

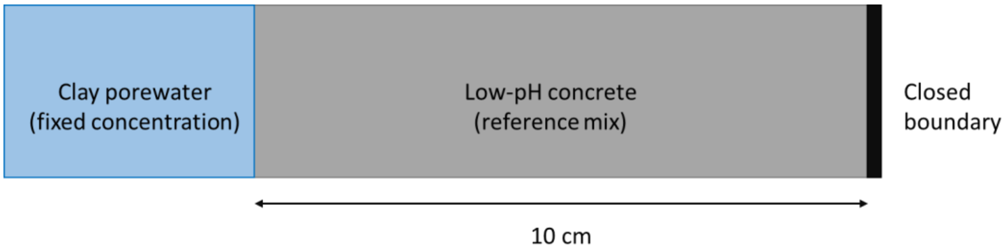


***Figure 1.*** *Schematic description of the application case.*

Details of the numerical techniques (spatial and temporal discretization, numerical scheme, etc.) depend on each modelling approach and will be discussed in the next workshop. Boundary conditions are fixed concentration (Dirichlet type) on the left of the concrete slab and no flux on the right.

The simulation time will be set to 10,000 years, which is based on an *a priori* estimation of the degradation of a 10-cm concrete slab with an effective diffusion coefficient of $3\cdot10^{-12}$ $m^2/s$.

### 3.4 Upscaling of the results

As stated above, some of the partners in WP3 do not develop models at the decimetre scale but focus on pore-scale and micro-scale processes. In that case, the implication of these partners (BRGM, JUELICH, SCK) will be to provide results at lower scales and upscaled estimates of porosity and transport properties for the intact material and for different levels of interaction with the clayey porewater. The implications of these results on continuum models at the decimetre and macroscopic scales will be discussed.

Moreover, the upscaling of the results of the application case at decimetre scale to repository conditions will also be considered in this sub task.

## 4 SCHEDULE

The planned schedule of the common modelling task is to start the activities during the 2nd Annual Workshop in May 2017. All the details of the simulation test case and the input data from characterization of the reference mixes in WP1 will be set, and the contribution of the different partners to the subtasks 1 to 4 will be defined.

Preliminary results of the first 3 subtasks will be presented in the 3rd Annual Workshop. The final results and conclusions of the first 3 subtasks together with the feedback from upscaling will be presented in the 4th Annual Workshop and described in more detail in Deliverable D3.07 “Report on the Upscaling Modelling Task” (M45, i.e. end of February 2019).