BELBaR D1.1

DEFINITION OF THE RELEVANT TYPE OF PARAMETERS SELECTED FOR EXPERIMENTAL AND MODELLING WORK

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1 Introduction

In the BELBaR description of work it is stated that WP1 will have the responsibility to ensure that the type and values of the parameters selected for experimental and modelling work should be those that will enable, as far as possible, representation of the range of different situations which can be expected in a repository. WP1 will define these parameters and values in an internal report at the beginning of the project – the current document. This report will be submitted to the end user review board for review and agreement with the consortium. This review and agreement will be a project milestone prior to engaging in core project work. This is done according to the information flow chart shown in Figure 1. The primary purpose of this document is to give a first indication of the content of the arrows leaving WP5. The arrows from WP5 represent the sub-chapters in the document, more information of the detailed input from safety assessment will be found in BELBaR deliverable D1.2.

The parameters measured in and obtained from the experiments will either be used to "validate" the quantitative models that are used in performance & safety assessments or to advance the conceptual (and mathematical) models. Already at this stage there is an idea to make a distinction between these types of parameters, even if there may be situations where they are overlapping.

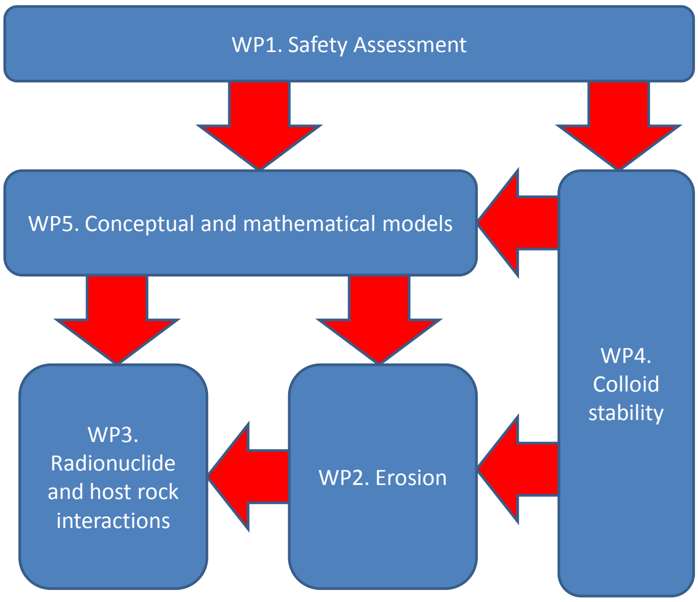

Figure 1 Simplified figure of the information flow between the work packages at the onset of the project

In BELBaR two principal processes of potential importance for the long term performance of a nuclear waste repository are studied: Erosion of a bentonite buffer and radionuclide transport mediated by bentonite colloids. The approaches for the handling of these two processes in safety assessments are different in nature and the parameters needed for their representation will be different. Therefore, the discussion on the parameter need has been divided into two separate sections:

2 Erosion of a bentonite buffer

The risk of buffer erosion has been defined to result mainly from the interaction with very dilute groundwater. The key factors to study is the conditions that lead to an onset of erosion and the the consequent mass loss rate. Therefore, one of the most important aspects to assess in the BELBaR project is to verify under which conditions onset of mass loss actually can occur:

The key factors study is colloid stability as a function of:

- Composition of the starting material
- Ionic strength
- Ion composition (mono- divalent)
- pH, edge charge

The second important aspect is the consequent mass loss rate.The BELBaR project does have a strong modelling component and both new model development and model extension are expected to take place during the project. However, as a starting point for the experimental targets the parameters in the current model used in quantitative assessments /Moreno et al 2010/ have been selected. This model calculates the mass loss as a function of water velocity and fracture aperture. The dominating control parameters in the experiments are then water flow rate and erosion geometry. The parameters needed for this model should be of importance for alternative models and model extensions as well. However, additional parameters may also be required and obtaining those should not be impossible, since BELBaR main is focussed on flexible, short duration tests.
The measured parameters for the validation of the quantitative models could then be:

1. Total mass loss rate
    - The value of this "variable" having a direct influence on a safety function indicator should be appropriately normalized to enable comparison between tests, e.g. as per unit area, but consideration is needed of the area used for normalization in radial geometries, i.e. what area is actually "exposed" to a conductive fracture?
2. Clay/gel penetration distance into a fracture
    - With respect to the initial position (or maybe absolute penetration distance in axi-symmetric setup?)
3. Density as a function of distance from the original position: the properties of the material as it penetrates into a fracture:
    - From what can be considered as bulk material
        - in the intersecting fracture case this is the same as distance from deposition hole and the setup is axi-symmetric and
        - in 1D-setups (like column tests) this will be the only running coordinate
4. Solids characteristics in the effluent
    - Colloids size and concentration
    - Exchangeable-cation composition??
    - Demixing of components in the solid Particle size distributions of both accessory minerals and smectites.
        - at the moment we can assess total mass loss *post mortem*
5. Chemical composition of the effluent (incl. electrical conductivity, EC)
    - Chemical composition of the final solution in the batch tests (incl. EC)

For advancing the model in /Moreno et al 2010/ and for the development of new approaches:

I. Clay/gel viscosity and Young's modulus (E' and E'' to characterize strength of the clay/gel)
    - As function of shear rates at low end, solids concentration, ionic strength, composition (homoionic and mixed solutions), pH, etc) This should be done also for cases where colloids are unstable.
    - The viscosity of dilute gel/sol of sodium montmorillonite in dilute homoionic solutions
    - It is highly recommended that bentonites with monovalent and divalent counterions will types of bentonite be included in the studies, as well as bentonites with a mixture of counterions..
    - The conservativeness in safety analysis by choosing Na-bentonite is probably valid for the mass loss criterion but not necessarily so from the erosion geometry perspective

II. Friction at clay-rock interface

- It is far less obvious how to handle this
- Surface roughness, could be oen alternative

III. interlayer spacing or other geometrical parameters like particle size, which is a valuable piece of information, these will have an effect on the colloid transport, especially diffusion, but it is not currently clear how this should be taken into account in developed models
   - Measurements of CEC, exchange complex, surface charge density and location, typical sizes of smectite particles in bentonites considered in BELBaR
   - Test parameters: solids concentration and porewater ionic strength

IV. The importance and appearance of accessory minerals
   - This includes complete characterization of mineral composition of MX-80, FEBEX or other bentonites considered in BELBaR
   - Experiments artificial or purified accessory minerals in an amount < 20% by mass, trying to make the accessory minerals identifiable or visible
   - Tests with variable amounts of accessory mineralsThe dissolution of gypsum and other calcium minerals contained in natural bentonite. The aim is to explore the effects of soluble minerals on the erosion of bentonite, as they may give rise to ionic strength above which destabilises colloids, before the time they have been fully leached from natural bentonite under repository conditions
   - Effects of salt dissolution on bentonite exchange complex
   - It is important to determine also the final solution composition, especially with batch tests.

V. Homogenisation of the deficit (due to mass loss)
   - Is as, if not more, important as the mass loss rate for penetrating copper corrosion. For example, the roughly same amount of corrodant from one intersecting fracture will corrode deeper (and make early through-penetration by corrosion) of the canister wall if the exposed area of the canister wall is smaller (with even lower mass loss)
   - The erosion geometry depends on the rheological properties of the yet not eroded mass (how effectively it will homogenise itself)
   - Ca- and Na-bentonite differs not only in that they will be chemically eroded at different rate, but also in that they homogenise themselves at rather different rates.
   - Some measurements of rheological variables of Ca-bentonite and mixed bentonites at low density may be needed
   - The homogenisation aspect is important, but it is not the key focus of BELBaR and it is studied in other projects. It is still anticipated that BELBaR may deliver some results with respect to the rheological properties of bentonite

VI. The importance and appearance of gravity
   - Experiments with inclined fractures as shown in Figure 2

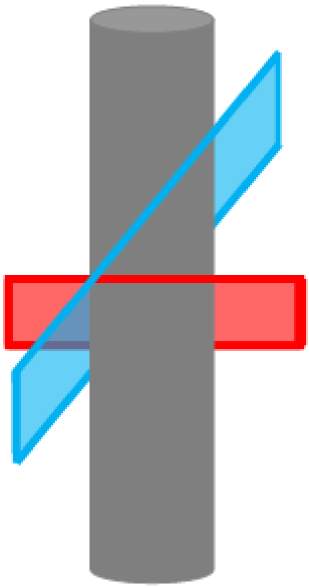

Figure 2 Inclining fractures intersecting a deposition hole

It is important to ensure that the initial state of any experiment is such that it enables as unequivocal an interpretation of the results as possible as decoupling of processes may often turn out to be very challenging, if not impossible. This pertains, for example, to the description of work under WP2:

> *"Experiments are initiated by **simultaneous** application of constant saturation head to the top and bottom of the samples and flow into the fracture ..."*

If the sample is not fully saturated initially, the experimental setup may not be representative of the issue *per se*. Would it be difficult to separate effects of bentonite saturation and concomitant extrusion and erosion by flow from each other, because application of a constant saturation head alone (without any flow) would make the bentonite saturate and extrude? If the experimental system is to simulate bentonite erosion at small scale, should the initial state in the experiment be such that bentonite has been let to saturate and extrude into a stagnant water-filled fracture prior to applying any flow?

3 Radionuclide transport mediated by bentonite colloids

When assessing the importance of radionuclide transport via bentonite colloids the following are proposed as the most important parameters:

- Near-field colloid concentration
- Near-field sorption distribution coefficients for sorption onto colloids
- Far-field colloid concentration
- Reversibility / irreversibility of sorption of radionuclides onto colloids (this is known to be of key importance, particularly in the far field)
    - Rate of sorption/desorption
- Colloid exclusion and other properties (sedimentation, coagulation, attachment to the fracture surface, etc.) that may affect the transport of colloid particles in the far field
- Surface charge on colloids
- Specific surface area of colloids

Depending on the outcome of modelling results based upon the above key parameters, it may also be of interest to increase understanding by exploring the following parameters:

- Far-field sorption distribution coefficients for radionuclide sorption onto inorganic colloids (i.e. the effect of sorption competition with natural colloids and rock surfaces)
- Sorption reduction factors due to organic complexants for sorption onto far-field colloids
- Colloid-rock distribution coefficients (i.e. potential attachment mechanisms for colloids onto rocks)
- Surface areas of porous rocks accessible to colloids (specific density of sorption sites).
- Implementing cation exchange processes to link surface charge effects on attachment probability and model with this approach the chemical effects on colloidal facilitated transport.

The choice of radionuclides for experimental work will be important. We note that the radionuclides most likely to be an issue due to colloid transport are those radionuclides that do not generally emerge in the biosphere due to strong sorption in the geosphere. These radionuclides include plutonium, neptunium, uranium, radium and technetium (IV). We suggest that the experimentalists propose the metal ions for this work for agreement by the Waste Management Organisations.

Useful information, albeit with a focus on colloids in an ILW system, is contained in a report produced by AEA Technology for Nirex /Swanton et al 2000/. The key area for PA model development is therefore likely to be irreversible sorption of radionuclides to colloids, should this be shown to be important.

4 References

Moreno L, Neretnieks I, Liu L, 2010. Modelling of erosion of bentonite by gel/sol flow. SKB TR-10-64, Svensk Kärnbränslehantering AB.

Swanton S W, Atkinson R, Sinclair J E, Poole M J, 2000. Calculations of the Potential Impact of Colloid Transport on Repository Performance. AEAT/R/ENV/0222.