WP FUTURE
Fundamental understanding of radionuclide retention

Dirk Bosbach/FZJ, Berlin, 3-4 December 2018

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FUTURE - Main Objectives

- Fundamental insights into the impact of chemical boundary conditions and the role of microstructures on radionuclide speciation and mobility in **"real" clay rocks as well as crystalline rocks**
- Enhance the quantitative and mechanistic understanding of the impact of (i) specific surface properties of materials (diffusive double layer, surface potential), (ii) the role of grain boundaries, (iii) the effect of water saturation, content and chemistry (pH, ionic strength) as well as (iv) the impact of pore size variability and heterogeneity on the mobility of chemical species
- Refined understanding of the relation between **fracture/ pore structures and transport as well as the feedback of mineral reactions** (dissolution/ precipitation) on solutes retention and transport.
- Closing knowledge gaps regarding **sorption reversibility, uptake mechanisms (adsorption vs. incorporation, precipitation), sorption competition and surface diffusion** which have not been addressed sufficiently in previous European projects (e.g. FUNMIG, SKIN).
- **Fundamental understanding and thus reducing uncertainties of surface induced (heterogeneous) redox processes with regard to coupled sorption and electron transfer interface reactions** governing the retention of redox-sensitive radionuclides at Fe(II)/Fe(III) bearing minerals surfaces – going beyond previous European projects (e.g. RECOSY).

FUTURE - Expected impacts

- **Provide the scientific basis needed to bind the applicability range and to estimate uncertainties in the simplistic concepts used in the current safety assessment (SA) studies**.
  - The development of multicomponent mechanistic sorption models and pore scale simulations of radionuclides transport will allow validation of the concepts used in SA and ensure that all relevant processes are sufficiently understood and are taken in to account in SA at an appropriate level, e.g. surface diffusion, sorption mechanisms, competition and reversibility in clay rocks. Moreover, the proposed research will contribute to the understanding of transport of radionuclides in the crystalline rock environment by properly identifying relevant properties and species involved in sorption and transport processes, altogether with description of fractured rock environment. The combined analysis of reactivity, structure, flow field, and RN mobility/ retention would provide a unique dataset that would enable to include local boundary driven transport processes into safety assessment models.
- The **R&D covers a substantial fraction of the sub-domains addressed in domain 1.6 Radionuclide and Chemical Species Migration of the SRA** regarding knowledge gaps related to sorption process, heterogeneous redox processes and in particular overall radionuclide mobility in "real" systems.
- **Link to the Roadmap Theme 4** (geoscience to understand rock properties, radionuclide transport and long-term geological evolution) phases 2-4.
- Improvement of the scientific basis for the safety case of deep geological disposal in clay rock and crystalline rock. **Reduction of uncertainties and potential reduction of conservatisms in more realistic descriptions of repository system evolution**.

FUTURE Participants

Organisations
✓ **Andra**, France (WMO) ▪ BRGM, France
✓ **CEA**, France (RE)
✓ **CIEMAT**, Spain (TSO)
✓ **CNRS**, France (RE) ▪ UGrenoble, France ▪ Upoitiers, France
✓ **FZJ,** Germany (RE) ▪ HZDR, Germany
✓ **GRS,** Germany (TSO)
✓ **KIT**, Germany (RE) ▪ JGU (UMAINZ), Germany

Organisations
✓ **MTA EK**, Hungary (RE)
✓ **POSIVA**, Finland (WMO)
✓ **PSI,** Switzerland (RE)
✓ **RATEN**, Romania (RE)
✓ **SURAO**, Czech Republic (WMO) ▪ UJV, Czech Republic
✓ **SCK-CEN,** Belgium (RE)
✓ **TNO,** Netherlands (RE)
✓ **UHELSINKI**, Finland (RE)

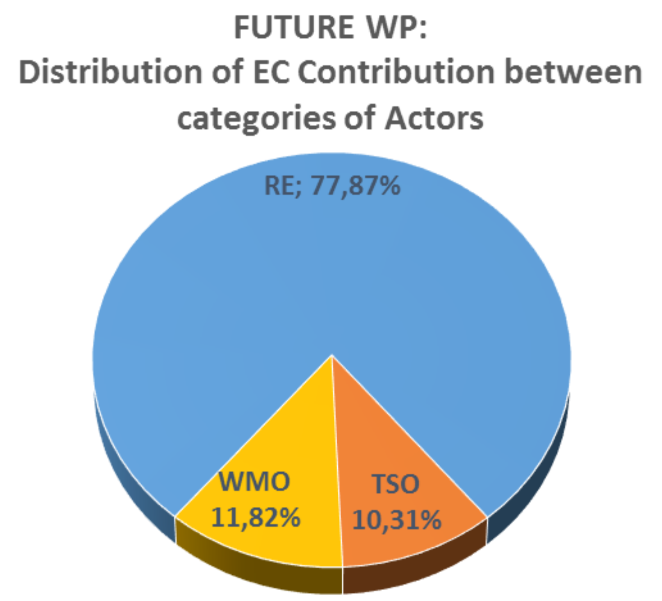
FUTURE – Task Breakdown and WP Board

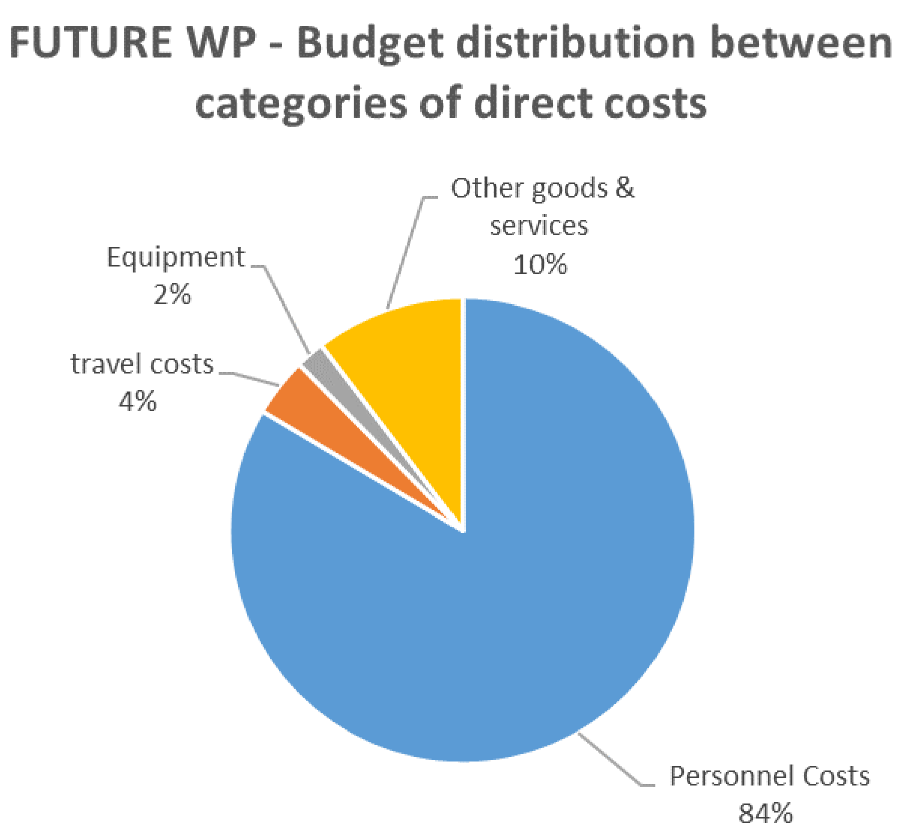
- Dirk Bosbach (d.Bosbach@fz-juelich.de)
- Vaclava Havlova (Vaclava.Havlova@ujv.cz)
- Sergey Churakov (sergey.churakov@psi.ch)

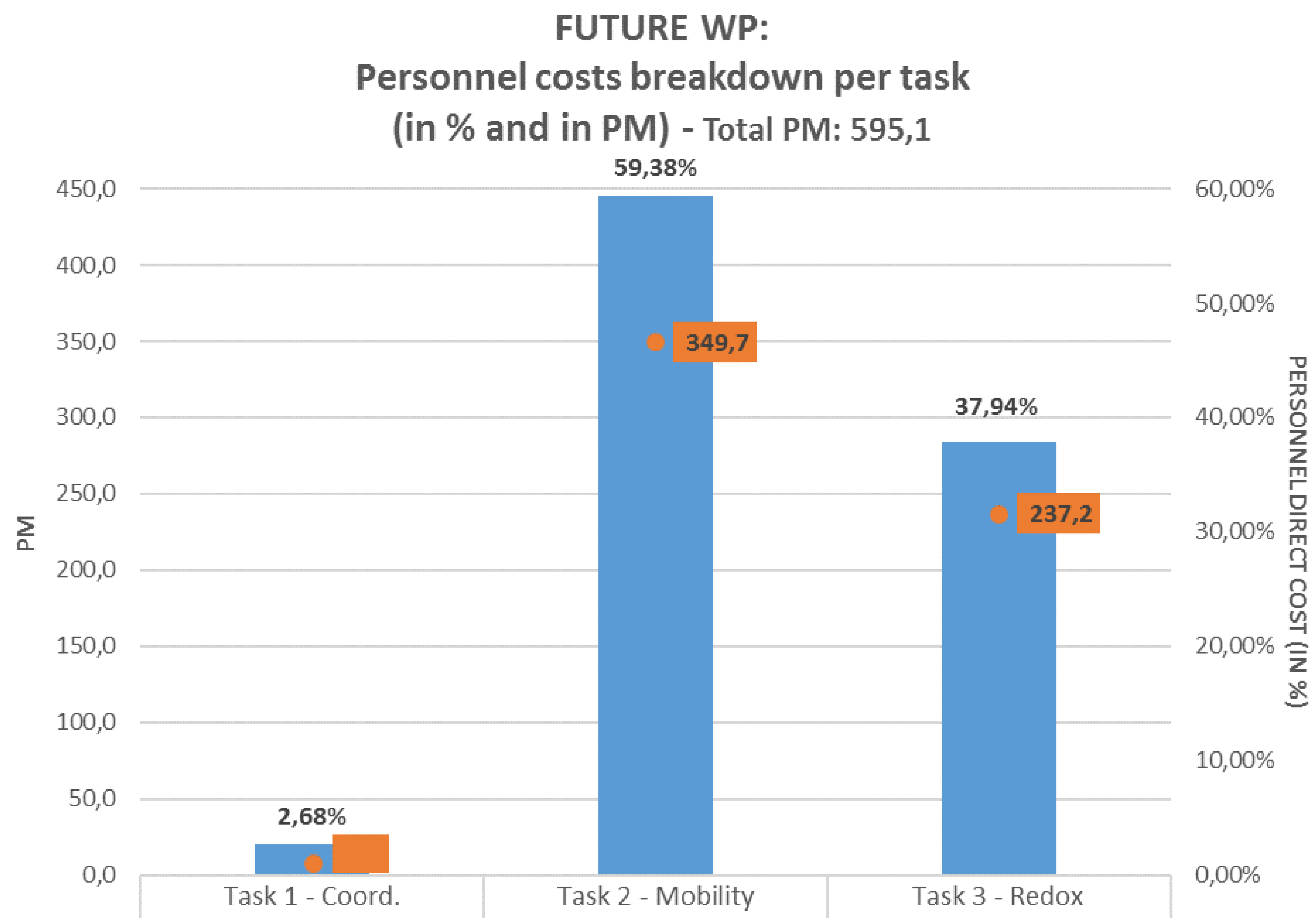
- **Task 1 - S/T coordination, state-of-the-art and training material**
  - Leader: Dirk Bosbach (FZJ)
- **Task 2 - Mobility**
  - Leader: Luc van Loon (PSI), Cornelius Fischer (HZDR), Norbert Maes (SCK.CEN)
- **Task 3 - Redox**
  - Leader: Sylvain Grangeon (BRGM), Marie Marques-Fernandes (PSI)

FUTURE – Planned resources

TOTAL BUDGET	4,6M€
EC requested contribution	2,3M€







FUTURE – Task 1 Coordination

- S/T coordination, State-of-the-art and training material
  - In order to set a "baseline" and as input to WP11-KM SoK, a **state-of-the-art report will be drafted at the start of the project** (Month 6) with the aim to provide a comprehensive overview of the available knowledge on the understanding of **radionuclide retention in clay and crystalline rocks** (D5.1). Emphasis will be on the current available knowledge with respect to i) **transferability of sorption phenomena to compacted/realistic systems and sorption reversibility** and, ii) **surface induced (heterogeneous) redox processes**.
  - At the end of the project (Month 48), this **report will be updated** incorporating the newly acquired knowledge (D5.2).

FUTURE – Task 2 - Mobility

- **Experimental studies on RN mobility in compacted clay** with strongly sorbing RN: actinides, intermediate sorbing RN: Fe, Ra, weakly sorbing RN: I/Se) and a limited number of clay systems: **pure clay systems (illite, montmorillonite) and clay rocks (in particular Opalinus clay and COx)**

- **Experimental studies on RN mobility in crystalline rock** with strongly sorbing RNs: actinides, intermediate sorbing RNs: Ra, weakly sorbing: I/Se): Identification of the impact of structure (connected pore network and surface topography of fractured crystalline rock samples and mineral infills) on RN mobility; impact of flow velocity; providing an interface to the WP4-DONUT (smart Kd approach) by using the quantitative information about parameter variability (surface charge, nanotopography, flow velocity anisotropy) that reflect the complexity of natural materials.

- **Sorption studies (excluding redox processes) with a focus on reversibility to close specific knowledge gaps** with Ni and Ra in support of mobility studies

FUTURE – Task 3 Redox reactivity of radionuclides on mineral surfaces

- Contribute to a better understanding of the **coupled sorption and electron transfer interface reactions** governing the retention of redox-sensitive radionuclides on Fe(II)/Fe(III) bearing minerals so as to improve our capacity to model, and thus predict, the fate of these elements within the safety assessment of radioactive waste storage.

- The interaction between different **redox–sensitive radionuclides** (or their non-radioactive analogues), including U, Pu, Tc, Np and Se, and **purified relevant Fe-containing minerals** and, to a minor extent, with rock envisioned as potential host-rocks (e.g., Callovian-Oxfordian) will be systematically investigated. Mineral properties with respect to its redox reactive iron content (structural/adsorbed) (i.e. abundance, location in the crystal structure, and oxidation state(s)) will be correlated to the degree of radionuclides retention (Kd) and molecular scale surface speciation.

- **The transferability of the knowledge gained on dispersed pure phases (batch experiments) to the description and understanding of diffusion processes of radionuclides in compacted systems will be verified.**

Key challenges & objectives for Year 1

- To start and develop communication and cooperation within clusters of institutions within Tasks
- organize a kick off meeting
- State of the art report
- The very first scientific activities, e.g. sample selection & preparation for further examination and experiments. Looking for the best initial samples will probably be one of the main tasks for the first year of the redox task
- Radionuclides and rock type matrix and distribute the load/activities between the labs
- Agree on experimental protocol/materials