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DELIVERABLE (D-N°:3.2) Availability and needs for technical and scientific tools for TSO's

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Sustainable network of Independent Technical Expertise for Radioactive Waste Disposal



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1 Content

1	Content			
2	Fore	word	7	
3	Sum	mary	7	
4	Intro	oduction	8	
5	Expe	erimental installations	9	
	5.1	Belgium	9	
	5.2	Canada	11	
	5.3	Czech Republic	13	
	5.4	France	20	
	5.5	Germany	30	
	5.6	Lithuania	32	
	5.7	Netherlands	32	
	5.8	Slovakia	34	
	5.9	Summary	35	
6	Mod	elling capacities	38	
	6.1	Belgium	38	
	6.2	Canada	40	
	6.3	Czech Republic	41	
	6.4	France	41	
	6.5	Germany	45	
	6.6	Lithuania	47	
	6.7	Netherlands	50	
	6.8	Slovakia	55	
	6.9	Summary	55	
7		ermination of capabitility to cover R&D needs for knowledge, identified e D3.1	58	
	7.1	Quality of input data	59	
	7.2	Understanding of Complex processes	61	
	7.3	Verification of extent, intensity and impact of processes	69	
8	Cate	gorisation of scientific issues	73	
	8.1	Quality of input data	74	



Sustainable network of Independent Technical Expertise for Radioactive Waste Disposal



	8.2 8.3	Understanding of Complex processes Verification of extent, intensity and impact of processes	75 78
9	Concl	usions	80
10	Refer	ences	81





Abbreviations

AAS	atomic absorption spectroscopy
ALARA	as low as reasonably achievable
ANDRA	National radioactive waste management organisation (France)
BN	Bitumen-Nitrate-Clay experiment
CARP	Coordinated Assessment and Research Plan
CCRMP	Canadian Certified Reference Materials Project
CEA	French Alternative Energies and Atomic Energy Commission
CEC	cation exchange capacity
CEG	Centre of Experimental Geotechnic, Czech Technical University, Prague
CEMTEX	Cement Temperature Experiment
CLINITEX	Cement-Interaction experiment
CNSC	Canadian Nuclear Safety Commission
CTU	Czech Technical University in Prague
DGD	deep geological disposal
DGD DGR	
EDZ	deep geological repository excavation disturbed zone
EBS	engineered barrier system
EBS	engineered barrier system
ELI	Ministerie Van economische Zaken, Landbouw en Innovatie, Netherlands
ETSON	European Technical Safety Onrganisation
FANC	Federal Agency for Nuclear Control, FANC, Belgium
FEP	Features, Events, Processes
FRACTEX	FRACture Transport EXperiment
GD	Geochemical data experiment
GD	geological disposal
GRS	Gesellschaft für Anlagen-und-Reaktorsicherheit, GRS, Germany
GTS	Grimsel Test Site
GUDS	Geologický ústav Dionýsa Štúra, Bratislava
HLW	high level waste
IAEA	International Atomic Energy Agency
ICP-MS	inductively coupled plasma mass spectrometry
ILW	intermediate level waste
IRF	instant released fraction
IRSN	Institut de Radioprotection et de Sûreté Nucléaire, France
LEI	Lietuvos Energetikos Institutas, Lithuania
LLW	low level waste
LTD	Long term diffusion project
MELODIE	Model for Long Term Assessment of Radioactive Waste Repository
MICADO	Module Internet de Calcul de Dose
MMSL	Mining and Mineral Science Laboratories
NEA	Nuclear Energy Agency
NRG	Nuclear Research and consultancy group, Netherlans
OECD	Organisation for Economic Co-operation and Development





OXITRAN	Oxidising transient
PA	performance assessment
PAMINA	project Performance assessment methodologies in application to guide the
	development of the safety case
PC-C	Porewater Chemistry Gas experiment
PCCS	photon cross-correlation spectroscopy
РСТ	product consistency test
PFAT	PetroFabric analysis of the Toarcian Argillite of Tournemire
R&D	research and development
RAWRA	Radioactive Waste Repository Authority
SEALEX	Sealing experiment
SEM	scanning electron microscopy
SITEX	Sustainable network of Independent Technical Expertise for Radioactive Waste
	Disposal
SNF	spent nuclear fuel
TEM	through-electromigration experiment
THM	thermo-hydrauli-mechanical
тнмс	thermo-mechanical-chemical
TIC	total inorganic carbon
TNO	The Netherlands Organisation for Applied Scientific Research
тос	total organic carbon
TSO	technical support organization
XRD	X-ray diffraction
URL	underground research laboratory
WIPP	Waste Isolation Pilot Plant





2 Foreword

The objective of the FP7 program SITEX project coordinated by IRSN, is to set up a network capable of harmonizing European approaches to technical expertise in of geological repositories for radioactive waste. Lasting 24 months, SITEX brings together 15 organisations representing technical safety organisations (TSOs) and safety authorities, as well as civil society outreach specialists.

SITEX plans to help establishing the conditions required for developing a sustainable network of technical safety experts who have their own skills and analytical tools, independently of the operators, and who are capable of conducting their own research programs in coordination with research activities performed by operators.

3 Summary

This report describes the tools (experimental installations, modelling capacities) that are already available to carry out expertise functions of technical safety organizations (TSOs) in the framework of reviewing safety of deep geological repositories. Furthermore, it aims to determine those that should be developed in order to improve TSOs capabilities in performing their R&D programmes.

The list of available labs and installation in countries, taking part in the Task was compiled. It revealed the fact that clear that some of the research areas are well covered (geochemical and geo-mechanical labs, modelling of transport and safety assessment etc.) Those are the topics, covering namely generic issues. Conversely, some of concept/site specific issues need to be either developed or the available resources are missing (study on bitumenised waste, influence of biota on corrosion, influence of defects etc.). However, the list of topics has been compiled on the basis of available resources of countries, participating in the WP3. The list would be different in case the structure of countries, involved in TSO's network change

Basically, the number of installations and tools available for a specific topic would decrease with increasing level of specificity. High-level scientific installations and labs require advanced and comprehensive maintenance. The same case appeared with advance code/models for specific topics. Therefore not all institutions can effort to develop them and maintain them. The straightforward examples are radiochemical laboratories and underground labs as specialized facilities with specific rules. Moreover, some of the installations are missing at all, for example underground laboratories in crystalline rocks that are mostly owned or facilitated by the implementers (Grimsel, Äspö, Oikiluoto, Horonobe, etc.). Such installations should be either shared in case they are available within "independent" circle or joint projects with other institutions, including WMOs, should be launched. In the last case the governance on the joint research activities is requested.





4 Introduction

The main role of technical safety organizations (TSOs) and their safety authorities is to provide independent review of safety cases prepared by operators and to help stakeholders, and particularly people from host communities, to trust in the waste management system. Their role in the service of people needs to be professed, verified and understood. The processes occurring in geological repositories are very complex and not yet fully understood. To get a deeper understanding of them TSOs must develop own scientific capabilities through systematic R&D programmes.

This WP3 is related to the development and maintenance of updated and independent scientific capabilities of TSOs or duly appointed bodies to perform independent technical assessments, by encouraging joined research and scientific and technical exchanges between TSOs and regulatory authorities as well as with operators at the European level.

The main aim of this deliverable is to identify the tools (experimental installations, modelling capacities) that are already available to carry out expertise functions of technical safety organizations (TSOs) and their safety authorities in the framework of reviewing safety of deep geological repositories. Moreover, the missing capacities should be identified in order to be developed to improve capabilities in performing their R&D programmes.

The following organizations are participating in on this deliverable:

BELV, Belgium Canadian Nuclear Safety Commission CNSC, Canada DECOM SA, Slovakia Federal Agency for nuclear Control, FANC, Belgium Gesellschaft für Anlagen-und-Reaktorsicherheit, GRS, Germany Institut de radioprotection et de Sûreté Nucléaire, IRSN, France Lietuvos Energetikos Institutas, LEI, Lithuania Ministerie Van economische Zaken, Landbouw en Innovatie , ELI, Netherlands UJV Rez, a.s. , Czech Republic





5 Experimental installations

5.1 BELGIUM

FANC and Bel V, constituting together the Belgian Regulatory Body, have both an important effort in R&D. By means of periodic meetings, FANC and Bel V keep each other mutually informed about on-going and planned R&D activities and participations.

The R&D activities of Bel V are primarily related to the development and the maintenance of expertise in nuclear safety and to a lesser extent in radiation protection (the latter being covered extensively by FANC). Within the framework of radioactive waste disposal safety, Bel V develops modelling capabilities for supporting the review of safety cases and has participated in international projects like 6th FP EC MICADO and 6th FP EC PAMINA (See section 6.1 for more details). Recently, the overall R&D effort foreseen by Bel V has been significantly increased to about 10% of the total available time for the technical staff. This additional effort will be notably devoted to supporting or participating in experimental R&D activities for the safety of radioactive waste disposal facilities. Regarding the safety of geological repositories, Bel V will develop an R&D programme based notably on the key issues identified in section 5.1 of the SITEX deliverable 3.1 [1]. Since Bel V does not have experimental installations, collaboration with other TSO's, Universities and research centres is envisioned for these R&D activities.

FANC contributes to the development and follow-up of various R&D activities in the frame of *in situ* experiments performed at the Mont Terri rock laboratory (CH) through a collaboration agreement with the Mol Nuclear Research Centre (SCK•CEN), the Belgian partner of the Mont Terri project since the beginning.

Key issues are identified on the basis of safety functions: physical containment of the waste, delaying and spreading in time the released radionuclides, limitation of water flow, and how to ensure stable conditions or to minimize perturbations. These issues are mainly associated to the processes on which rest the safety functions and the potential perturbations that may compromise the long-term safety of the repository. Technical issues are also associated to the methods of acquisition of key data on the host-rock and on the Engineered Barrier System (EBS), and to the modelling of the long-term radiological impact of the waste disposal facility.

The *in situ* experiments whose SCK•CEN is partner at Mont Terri and co-supported and followed by FANC are listed in Tab. 1 as a function of the priority for R&D needs for knowledge identified in the section 5.1 of the SITEX deliverable 3.1 [1].





Key issues	R&D needs	Mont Terri experiment
Data acquisition	Development of methods to characterize the host rock formation	PC-C : Porewater Chemistry Gas (pCO ₂ , pH, E _h)
		<u>GD</u> : Geochemical data: follow- up of the porewater geochemistry in various boreholes and in situ experiments
Long-term stability: Internal perturbation	Waste / host-rock interactions - Nitrate plume - Clay oxidation - Microbial activity - Gas generation (N ₂)	<u>BN</u>: Bitumen-Nitrate-Clay experiment
	EBS / Host rock interactions - Alkaline plume - Cement degradation	<u>Cl</u> : Cement-Interaction

Tab. 1. Mont Terri experiments supported by FANC through collaboration with SCK•CEN

The aims and the motivation of the PC-C, GD, BN and CI experiments at Mont Terri are summarized hereafter.

5.1.1 PC-C: Porewater Chemistry Gas (pCO₂, pH, E_h)

As stressed by the NEA peer review committee for the SAFIR 2 report, the partial pressure of CO_2 is a key parameter to constrain the carbonate system and the pH of the porewater of the host rock. These geochemical parameters are essential to understand and to predict the speciation and the solubility of radionuclides and to underpin their migration studies (sorption behaviour, diffusion parameters...). The first aim of the PC-C experiment is the *in situ* monitoring of the evolution of the gases composition (mainly CO_2 , but also CH_4 , C_2H_6 and N_2) at equilibrium with porewater and the water sampling under a protecting gas phase. A second objective is to test online measurement systems (pH and E_h electrodes in flow-through cells).

5.1.2 GD: Geochemical data

The aim of this project is to follow the evolution of the porewater chemistry in various boreholes and *in situ* experiments at Mont Terri and to build a database that can be used for geochemical modelling. In parallel, unresolved issues dealing with the geochemical porosity of highly compacted clay formations and geochemical interactions are also addressed in the frame of this project.

5.1.3 BN: Bitumen-Nitrate-Clay experiment





The BN experiment aims to investigate the combined reactivity and transport of a plume of nitrate and bitumen degradation products and its biogeochemical effects on the near-field host rock, including the transport of redox-sensitive radionuclides (*e.g.*, ⁷⁹Se, ⁹⁹Tc, ^{23x}U, ...). The results obtained by the BN experiment are also relevant to the PC-C and GD projects.

The BN experiment has been designed to simulate conditions prevailing in the clay host rock surrounding a bituminised, or other nitrate-bearing waste cell. To make abstraction of complex interactions with cement in the near-field, the initial focus of the BN experiment is to study the effects of a Nitrate/Bitumen Degradation Product plume (organic matter, OM) on the argillaceous host rock only. Accordingly, bio- and geochemical interactions between the nitrate/OM plume and the clay are studied under natural to slightly alkaline conditions (anticipated pH: 7-9), expected in the excavation disturbed zone (EDZ) at some distance from the cement/clay interface. Under these pH conditions, likely initial inhibition of microbial activity and alkaline plume related mineralogical changes are avoided. Higher pH conditions (pH: 9-11) will possibly be investigated further in view of studying the behaviour of alkaliphilic microorganisms, which might be active in a real cement-dominated storage environment. The BN experiment consists of two parts: the field test and lab supporting experiments.

5.1.4 CI: Cement-Interaction

The purpose of this experiment is to study on the long-term (up to 20 years) the interactions between cement and the clay host rock or bentonite materials. Various types of cement (OPC, low pH cement...) intercalated by different bentonite plugs have been installed in two boreholes drilled under controlled conditions and subsequently saturated with synthetic Opalinus Clay water. At different times (2, 4, 8, 16,... > 20 years, ...) oblique boreholes are (or will be) drilled in order to intersect different cement/clay interfaces in the two test boreholes. A new overcoring technique recently developed by Bern University was successively tested in February 2012 and allowed to retrieve very well preserved samples to characterize the evolution of minerals and porosity at the interface concrete – clay using classical techniques (XRD, TGA, SEM, TEM, NMR, ¹⁴C-autoradiography, ...) and advanced synchrotron methods (μ -XRD / μ -XAS). The *in situ* boreholes are accompanied by mock-up samples consisting of OPA cores and bentonite plugs embedded in concrete made of OPC and low-pH cements also stored in the rock laboratory.

5.2 CANADA

5.2.1 CNSC Laboratory

CNSC has a modernized laboratory that substantially enhances the CNSC's capability to verify licensee compliance programs in radiation protection, environmental protection, safeguards, and emergency preparedness. In addition, the laboratory is increasingly engaged in research and collaborative activities with various national and international partners on subjects that are of high significance to the CNSC's regulatory regime.

The laboratory includes the following featured rooms: Gamma Irradiator rooms, Neutron Irradiator, Environmental Sample Preparation Room, Analytical Instruments Room,





Environmental Counting Room, Wet Chemistry Laboratory, Radiological Counting Room, Clean Room, Matrix Preparation Laboratory, and Dispatch Room.

5.2.2 CANMET Mining and Mineral Sciences Laboratories (MMSL)

CANMET Mining and Mineral Sciences Laboratories (CANMET-MMSL) is one of the Canadian government laboratories at Natural Resources Canada (NRCan), which is the primary source of scientific research and advice on mining and mineral technology for the mining and minerals industries as well as the provincial, territorial and federal government departments that promote or regulate these industries. CANMET-MMSL also provides laboratory services to other industries and organizations to promote the scientific advancement and improve the industry practical performance.

CANMET-MMSL researches and develops processes and technologies involved in extracting ore from the ground and transforming it into a concentrate, mineral product or metal. CANMET-MMSL has a long-standing international reputation for technical excellence in mining and mineral processing and is a recognized leader in the development of technological means of reducing environmental impacts and improving mine workers' health and safety.

CANMET- MMSL is a market-oriented organization that is responsive to industrial and national needs. Success is measured in terms of the strong level of support by the client community, and by the impact of CANMET-MMSL's activities on industrial operations. CANMET-MMSL also provides expertise and services to mining and metals policy groups at NRCan, and other federal government departments through a MOU (Memorandum of Understanding), in order to strengthen the scientific input into policy and regulatory development.

CANMET- MMSL provides expertise and laboratory services under the following four groups:

The mining group specializes in the areas of:

- ground stability monitoring and control;
- mine mechanization/automation;
- mine air quality and ventilation; and
- coal mining health and safety.

The mineralogy and metallurgical processing group undertakes development in metallurgical processing, and minerals and metals recycling, and also provides support and carries out development in applied mineralogy.

The environment group specializes in the treatment of gaseous and liquid mine and mill effluents (including acidic drainage), mine decommissioning and rehabilitation, and provides scientific input in the development of environmental policies and regulations for metals.

The Canadian Certified Reference Materials Project (CCRMP) prepares and certifies reference materials principally for Canada's mineral metallurgical, earth science, and environmental industries. CCRMP also has a custom reference material preparation service and a lab proficiency testing program.

SITEX





5.2.3 Underground Research Laboratory

CNSC, as a Canadian nuclear regulator, has no underground research laboratories (URL) currently and has no intention to own one in the future. However, CNSC will collaborate with other organizations such as IRSN and others who own an URL for some R&D actions that are related to the nuclear waste management.

5.3 CZECH REPUBLIC

5.3.1 Experimental installations

Experimental installations of UJV in the field of radioactive waste disposal have been built primarily to get data for preparation of safety cases of existing near-surface radioactive waste repositories and planned deep geological repository. They can be divided into the following laboratories:

- 1) Laboratory for investigating host rock migration properties
- 2) Participation on in-situ experiments in real rock environment
- 3) Laboratory for investigating buffer and backfill materials
- 4) Laboratory for investigating waste and waste package materials

5.3.1.1 LABORATORY FOR INVESTIGATING OF HOST ROCK MIGRATION PROPERTIES

The laboratory for investigating host rock properties are focused primarily on investigation of migration properties of crystalline rocks as preferred candidate host rocks in Czech reference project of a deep geological repository. Research activities have been focused primarily on development facilities and methodologies for measuring diffusion and sorption coefficients of radionuclides in granite and investigating processes related to them. An important part of research activities is now focused to transfer our knowledge from laboratory experiments to experiments "in situ" that should use primarily for verifying the results obtained in laboratories. The following experimental facilities and methodologies have been developed in UJV for investigating granite migration properties:

Measuring sorption coefficients of contaminants in crystalline rocks under static conditions

Sorption of species on the crystalline rocks under static conditions is measured using the conventional batch sorption methodology. The methodology can be applied both for radioactive and non-active tracers. It uses simple approach of the batch reactor in which defined amount of solid matter and tracer solution are added. Activity/concentration development in the experimental solution is then observed, using appropriate solid/solution separation techniques and analytical tools for tracer determination in the samples. Sorption is usually studied using defined particle size fractions, ranging from fine ones up to coarse particles and/or rock pieces under different solid to liquid phase ratios and concentration dependence. Resulting sorption distribution coefficient is determined on the basis of ratio of tracer sorbed on the solid and tracer in the solution.

SITEX





Measuring sorption coefficients under dynamic conditions (column experiments)

Column experiments enable to study sorption properties of the rock material under dynamic conditions. Set up of column experiment usually consist of a vessel, packed with crushed material that is lined up with the solution reservoir by the peek lines. Different particle size fractions are usually used for the experiments. Solution is pushed by peristaltic pump through the rock column under defined conditions (namely flow velocity and volume). The content of tracer is determined, sampling the outflow below the column and by determination by appropriate analytical conditions. Tracer input can be accomplished in two ways. Firstly, the tracer pulse is injected i.e. a single-defined tracer amount is added into the head of the saturated rock column. The arrival time and shape of the resulting pulse is then studied. Secondly, the tracer solution is conducted through the rock column until full saturation. Resulting S-curve is then used for transport parameter determination.

Measuring diffusion coefficients in crystalline rocks

Diffusion coefficients are determined in UJV primarily using through-diffusion methodology, which is based on emplacement of the rock sample disc between spiked reservoir (in-let reservoir) and tracer free reservoir (out-let reservoir) and evaluation of growth of concentration of a contaminant in tracer free reservoir and using electromigration methodology that enable significantly accelerate diffusion process.

Through diffusion methodology

The rock sample is fixed in between the reservoirs using silicon based sealing that enables to use samples of different diameters (40, 46 and 50 mm). The sample thickness is usually 10 mm.

The tracer diffuses from the in-let reservoir through the rock sample. The increase of activity/concentration is determined in the out-let reservoir, analysing activity/concentration increase in samples, regularly taken from the out-let reservoir (experimental breakthrough curve). Prior to through-diffusion experiment the rock sample porosity is usually measured. Then the sample is saturated by solution that is used in out-let reservoir (usually synthetic groundwater). Two different approaches can be used: firstly transient boundary conditions when both in-let and out-let reservoirs are not kept stabile, i.e. activity decreases in the in-let reservoir and activity increase in out-let reservoir. Secondly constant boundary conditions when constant tracer content is held in both reservoirs. The first approach is more suitable for radioactive tracers, the second one for non-active tracers. Diffusion coefficient is then determined according to boundary conditions, using given mathematical solution.

Tracer content (activity, concentration) is determined according to tracer nature. Radioactive tracer concentration in the liquid samples can be determined using automatic gamma counter and automatic liquid scintillation counter. Non-active tracer concentration can be determined by mass spectroscopy, atomic absorption spectroscopy or electrochemical methods, depending on tracer concentration.





Through electromigration methodology

Through electromigration method (TEM) can be used as a complement method to the used through diffusion method or as an independent method, because electromigration experiments are less time-consuming then through diffusion experiments. When running the experiment, the tracer will migrate into the porous system of the rock with the electrical potential gradient as the main driving force. After some time, all transport pores of the sample will achieve approximately the same tracer concentration as in the high concentration tracer compartment (as opposed to the situation in a through diffusion experiment, where there will be a concentration gradient over the sample within the porous system).

In UJV own electromigration experimental apparatus has been developed based on the apparatus developed in Sweden [2]. In the centre of electromigration cell sealed rock sample is placed, connected to the high and low tracer concentration reservoirs. These two tracer reservoirs are connected to the two main reservoirs with basic electrolyte by filters made from granitic rock. To neutralise changes and decomposition of electrolyte by electrolysis, main reservoirs are cross connected and electrolytes are intermixed. To avoid current from being propagated in the hoses used for intermixing the anode and cathode electrolytes, stages of drop wise flow of the electrolytes are needed. The anode and the cathode are connected to a direct current power supply through an ampere meter. Electric potential on sample is measured by volt meter connected to potential electrodes. Electromigration is the main process of solute transport, the studied tracer should be ionic and in present time running experiments the non-radioactive iodide anion I- is used. The potential gradient over the sample could be achieved by placing an electrode in each electrolyte and connecting the electrodes to a direct current power supply. Nowadays the cell for measurement of samples of different length (10 - 100 mm) is available.

In-situ experiments in underground laboratories

The underground laboratories serves as an environment for testing phenomena observed in laboratories, the conditions in underground are closer to conditions in future deep geological depository than are those in a laboratory.

UJV have been participating in the long-term diffusion project (LTD Phase I. and II.) in Grimsel site in Switzerland for more than 5 years (www.grimsel.com). Recently it has also started in-situ experiments in underground laboratory JOSEF situated which was excavated as part of the exploration of local gold-bearing deposits. The research is focused now primarily on preparation of experiments and acquiring appropriate knowledge to conduct experiments confirming the results achieved in laboratories.

It is also planned to start experiments in underground laboratory Skalka situated near area used for uranium mining and near one of candidate sites selected in the Czech Republic for a deep geological repository. The underground laboratory is situated in an exploration gallery, whose intended role in the described locality is to serve as possible place for interim storage of spent nuclear fuel. The geotechnical and all geological conditions of the exploration gallery are very well described; the overlying rock thickness is about 100 m.





Facility for measuring hydraulic aperture of fractures

Facility for measuring hydraulic aperture of fractures is based on injection of water into isolated part of borehole under pressure of up to 5 atm. The pressure of injected water as well as the sensitivity of the flow meter is chosen according to expected fracture's hydraulic aperture. The principle of measurement consists in recording flow rate depending on pressure of the infiltrated water. The instrument contains a source of pressure water, a sensor of pressure, a mechanical obturator, a flow meter and a datalogger, which record the flow rate and the pressure of injected water. The sensitivity of flow meters is following: 0.1-2 I/ min, 0.5-7.5 I/min, 1-10 I/min, 2-35 I/min

Facility for measurement of materials with very low hydraulic conductivity

Facility for measuring very low hydraulic conductivity of host rock has the same principle as the measurement of fracture's hydraulic aperture with the difference that the source of pressured water and the flow meter are replaced by a volume meter. The volume meter contains a chamber with the volume of 1 litre and water is either pressed by piston's weight or the pressure of water can be controlled by pressure of air. The movement of the piston is recorded and it is recalculated to flow rate according to a calibrating curve.

The experiments can be carried out with any tracer (in our case with salted water) in order to find out the mutual boreholes' communication. The tracer arrival time is observed in the neighbouring boreholes. The fractures' hydraulic aperture is evaluated using the methods for injection test in a porous medium in combination with Hagen-Pouisell's law.

Planned facilities

For deeper boreholes it is planned to acquire a two-part obturator so that the selected fracture or selected parts of matrix could be examined individually. The continual observation of water level and of electrical conductivity of water in the neighbouring boreholes will be added to tracer exam dealing with fracture geometry. It is desirable to catch the whole breakthrough curve and not only tracer arrival time from the reason of overall balance of the tracer.

In the first in situ experiments under preparation, serving for verifying migration properties of crystalline rocks, the contaminant will be placed in boreholes in glass tubes, surrounded by bentonite that by swelling pressure will destroy the glass enabling it to migrate in bentonite and then to granite. After some time the borehole will be over-drilled and the concentration of contaminant will be determined. The results will be compared with modelling results.

5.3.1.2 LABORATORY FOR INVESTIGATING OF BUFFER, BACKFILL, PLUGGING AND SEALING MATERIALS

In the Czech DGR concept buffer, backfill, plugging and sealing materials are based on bentonite and cement. The following experimental facilities and methodologies are therefore focused on investigation of these materials

Measuring sorption coefficients on bentonite under static conditions

For determination of sorption of species in the buffer, backfill plugging and sealing materials the batch methodology modified for swelling materials is applied in standard test with both





radioactive and non-radioactive tracers. Used equipment allows testing at various conditions of solid and liquid phase with possible identification of colloidal particles (their size, tracer content).

Measuring diffusion coefficients through compacted bentonite

Diffusion of species through the compacted buffer and backfill materials is complicated by swelling character of bentonite. Special diffusion cells able to withstand great swelling pressure and having very thin filters were therefore developed in UJV to study the diffusion of mobile species. Long term diffusion experiments with the species potentially interacting with a steel or other metals can also be performed because of the inner parts of the diffusion cell are made of carbon composite material. The length of the sample can vary in the range 5, 10 and 15 mm and can be simply adjusted by adding the inner part of the cell with required length. The 300 kN PC-controlled hydraulic press can be used for sample preparation matching the required parameters for the experiment (compacted dry density, sample length). For solid sample saturation, gas/liquid or gas/liquid/liquid pressure multiplier can be used to saturate the compacted samples at required constant pressure using various solutions. After the diffusion experiment, compacted saturated sample can be divided into required amount of thin slices using a special cutter allowing to obtain slices with various thicknesses for later profile analysis. At the present time, following methodologies are used: through diffusion with diffusion coefficient evaluation based on tracer concentration decrease in input solution or tracer concentration increase in output solution (both radioactive and non-radioactive tracers can be used); through diffusion, the steady state method (non-radioactive tracers). The combination of both methodologies with the methodology of tracer profile evaluation in the compacted sample is in development.

The analytical facilities used for determination of tracers can be divided into two main parts for: 1) applications used in radiotracer determination and 2) applications used in non-radioactive determination. In the first case, automatic gamma counter and automatic liquid scintillation counter can be used according the type of the tracer. In the second case, depending on the tracer concentration, mass spectroscopy, atomic absorption spectroscopy or electrochemical methods can be used.

Investigating bentonite colloid chemistry

Clay colloid chemistry and the properties of bentonites and smectites have been studied intensively during a long time, both within and outside the waste management community. Nevertheless, there are areas where the behaviour of smectite gels and sols are not sufficiently understood.

Generally, the experimental investigations of bentonites in UJV include the chemical and mineralogical characterization, preparation and purification (to homoionic forms) and sorption studies with radionuclides (e.g. [4], [5]). For the characterization of colloids the new device using photon cross-correlation spectroscopy (PCCS) (NANOPHOX, Sympatec GmbH, Germany) was acquired. This technique allows the simultaneous measurement of particle size and stability of opaque suspension or emulsions of nanoparticles (colloids) in the size range of about 1 nm to some μ m. Because the clay colloid issue is still important in safety case, further work will focus on clay suspensions stability studies under different geochemical conditions, interaction of clay colloids with relevant radionuclides and also





erosion experiments mainly with Czech bentonites.

Investigating bentonite pore water chemistry

The knowledge of pore water composition is one of the key parameters for understanding and prediction the processes that will take place in the Deep Geological Repository. Generally accepted approach for studying porewater evolution is a combination of experiments, followed by the geochemical modeling and its comparison to experimental results. In UJV the geochemical modeling is performed in geochemical code PHREEQC2. The experimental techniques cover e.g. aqueous extraction under different V/m ratios, highpressure squeezing, cation exchange capacity and exchangeable cations determination. So far, our studies were focused mainly on Rokle bentonites (Rokle deposit, NW Bohemia, CZ, see [5]). Further, we would like to focus on techniques including porewater determination in granite microstructures i.e. granite porewater.

Measuring bentonite cation exchange capacity (CEC)

Determination of cation exchange capacity (CEC) is a common study method in soil science, but also one of the most important parameters of buffer and backfill materials in Deep Geological Repository concept. Standard methods to determine CEC use ammonium acetate (e.g. [7]) or barium chloride [6], but these methods are time consuming and in some cases give non adequate results for bentonite samples. Other methods using Cu/Ni amine complexes enable simple estimation of CEC and avoid some of the disadvantages of the standard methods. It should be also noted, that in comparing CEC values obtained by different methods (mainly differ in pH of cation exchange); possible method-specific systematic differences must be taken into account. Methodology of CEC measurement using Cu(II)-triethylentetramine is standard laboratory procedure in UJV [8]. Total concentration of Cu is measured by UV/Vis spectroscopy (Specord 205 – 222A358, Analytic Jena Co., Germany) or by AAS (SavantAA, GBC Scientific Equipment , USA), similarly as the exchangeable cations.

Measuring cement materials properties

Cement mixtures and concretes will be used as a matrix for solidification of wastes or as a construction material in waste repository. In many cases special cement materials with low pH should be used to avoid interactions with other materials of repository barriers which could negatively affect their properties.

In UJV mixtures of cement with other components to obtain mixtures with physical and chemical properties suitable for using in different areas of waste management are being developed. One of the goals is to develop mixture with low pH of leachate. Facility and methodology is available for measuring leachate pH measurements using internationally tested methodology and measuring compressive strength of cement samples.

5.3.1.3 LABORATORY FOR INVESTIGATION OF WASTE AND WASTE PACKAGE MATERIALS

Waste characterization and investigation of waste packages materials belongs to one of the subjects of research of UJV since sixties.





Facility for waste characterization

UJV has a number of experimental equipment for characterization of waste properties. Inventory of waste can determined both by destructive and nondestructive methods. A number of certified methodologies for determination of gamma, beta and alpha nuclides have been introduced as routine laboratory procedures.

The leaching of radionuclides from waste forms is investigated by ANSI/ANS 16.1 "measurement of the leachability of solidified low-level radioactive wastes by a short-term test procedure" or by Product Consistency Test (PCT). Since most of liquid, operational waste in Czech NPPs is bituminized, one of the research activities is long-term investigation of degradation and water uptake of bituminized waste.

Facility for investigating waste package materials

Following methodologies have been developed primarily for investigation of long-term corrosion of steel based materials under anaerobic conditions which should serve as materials of waste packages for spent fuel assemblies, but the same procedures are also applied for measuring corrosion properties of copper. For most of the experiments the corrosion cells are emplaced in an anaerobic box (MBrown, Germany) with an argon atmosphere and less than 0.1 ppm oxygen content. Special corrosion cells enabling to measure corrosion rate in contact with compacted bentonite have been developed.

Corrosion potential measurement

Measuring electrochemical methods in modeling bentonite pore water is possible by Gamry Instruments PC4/750 Potentiostat/Galvanostat/ZRA. This device can perform "standard" electrochemical corrosion techniques like potenciostatic/galvanostatic, voltammetry, cyclic voltammetry etc. It is also possible to measure electrochemical noise on the samples. PC4/750 potentiostat/galvanostat/ZRA can be used at aerobic conditions. Using this device at anaerobic box (concentration of oxygen under 0.1 ppm) it will be possible by upgrading system for signal transfer between device (outside anaerobic box) and corrosion chamber (inside anaerobic box).

Corrosion rate from weight loss measurement

Corrosion tests in modeling solutions can be performed in various corrosion cells. Devices are capable to control temperature of the experiments and whole equipment can be put inside the anaerobic box. Corrosion rate is evaluated from measuring weight loss of samples. Inside the anaerobic box it is possible measuring pH and redox potential directly in corrosion chamber or after sampling solution.

Hydrogen generation measurements

A special device has been developed for measuring hydrogen generation from corroded metals. This device allows hydrogen evolution to be continuously measured at different temperatures and at a constant pressure in the water. The source of pressure is a heavy piston, moving in mutually interconnected pressurized cylindrical vessels with a rolling membrane. The volume measurement is based on detecting the piston.

Special corrosion cells have been developed for measuring corrosion of metals in direct





contact between samples and compacted bentonite. Bentonite during the experiment is saturated by high pressure (50-100 bar). Whole apparatus contain of hydraulic part and corrosion cell with temperature regulation.

It also is possible to perform corrosion experiments in field of ionization radiation (source ⁶⁰Co) both under laboratory and elevated temperatures. Maximum applicable dose rate is 1 kG per hour.

A special in situ corrosion probes are now under development to conduct experiments in underground laboratories. The corrosion probes will enable to conducts experiment under elevated temperatures and in contact with saturated, compacted bentonite.

Corrosion environment measurements

Various types of both commercial and home-made electrodes (Pt, Au) are used to measure Eh and pH in the system with corroded metals. The concentration of Fe²⁺ ions in the solution after the experiments is measured by UV/Vis spectrometer by the modified ferozzine method sulphide by a Spectroquant test kit. The total iron concentration in the solution is measured by atomic absorption spectroscope Varian SpectrAA 200.

Nature of corrosion products is measured in cooperation with Czech Chemical Institute in Prague by Raman spectrometer LabRam (Horiba – Jobin Yvon, France) with two lasers (He – Ne and Ar), by X-ray diffraction Philips-Xpert PRO (PAnalytical, Netherlands) and by ESC Probe P (Omikron Nanotechnology, Germany) in the CAE mode (Constant Analyser Energy)

5.4 FRANCE

The French National Radioactive Waste Management Agency (ANDRA) is responsible for designing, constructing and operating a geological radioactive waste disposal facility. Pending approval, this facility will be opened in eastern France in 2025. With this in mind, Andra has been operating an underground laboratory in Bure (Meuse) since 1999, where it carries out studies and research. To ensure an independent assessment of Andra's project, IRSN has been carrying out for the past 20 years its own research in various experimental installations. The research carried out there has enabled IRSN to examine certain processes that play an important role in ensuring the long-term safety of a geological repository.

IRSN's different experimental installations can be divided as follows.

5.4.1 Laboratory of analyses and Experimental Resources (LAME)

The LAME is located on the CEA (Atomic Energy and Alternative Energies Commission) site of Fontenay-aux-Roses (10 km south of Paris); its principal missions are as follows:

- Carry out measurements for the physical, radiological, and chemical characterizations of soils, rocks, and waters;
- Develop and test physical, radiological and chemical characterizations methods for soils, rocks and waters;
- Contribute to define and implement experimental protocols in response to requests from bodies inside or outside IRSN;
- Acquisition, management, and maintenance, in compliance with regulatory





requirements and the procedures laid down by IRSN;

- Management support and maintenance of analytical and experimental resources deployed at the Tournemire underground experimental station and on the Chernobyl pilot site;
- Participate in a global network of metrology and also assist with the seismological and geodesic networks.

5.4.1.1 MAIN EQUIPMENT

The LAME laboratory has a monitored facility zone including an ICPE (classified installation for the protection of the environment), which enables the handling of radionuclides (HTO, ⁹⁰Sr, ¹³⁷Cs, ¹²⁵I, ²²⁶Ra, etc.) and the use of radioactive sources. The laboratory is equipped with chromatographic equipment (study of column migration under saturated conditions) and a gammametric test bench (column migration under unsaturated conditions).

5.4.1.2 ANALYTICAL RESOURCES

Among the available analytical resources, the ones directly linked used in the frame of GD expertise are:

- Soil characterisation: laser granulometry, specific surface measurements by BET, optical microscopy and scanning electron microscopy (SEM) coupled with energy dispersive spectrometry (EDS);
- Solution characterisation: atomic absorption spectrometry, ion chromatography, ICP-MS, spectrophotometry, total organic/inorganic carbon measurement (TOC/TIC);
- Radiological characterisation of solids and solutions: gamma spectrometry, liquid scintillation, emanometry (radium measurement);
- Preparation of solid samples (thin sections, resin encapsulation, polishing, etc.) for observation and chemical analyses by SEM-EDS;
- Temperature controlled ovens, agitators, baths and cabinets, pH meters.

5.4.2 The Tournemire Underground Experimental Platform

Acquired by IRSN in 1992, the Tournemire experimental station, together with the Mol (Belgium), Mont-Terri (Switzerland) and Bure (Meuse, France) laboratories, is now one of the four underground laboratories in Europe carrying out research on disposal in clay formations. Located in a former railway tunnel built over 120 years ago, this station allows access to a clay formation that has similar geological characteristics to the site chosen by Andra in Bure (Meuse-Haute Marne).

The Tournemire experimental station is solely used for scientific and technical research. There is no intention of disposing of radioactive waste there at any time in the future. Furthermore, no radioactive components are brought to this site for the purposes of the research carried out here.

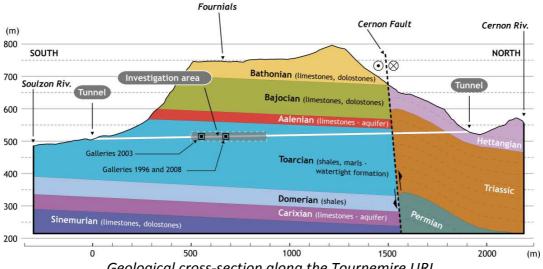
5.4.2.1 GEOLOGICAL AND TECTONIC FEATURES

Tournemire is located in the western part of the Causses Permo-Mesozoic sedimentary basin (SW France). The basin is surrounded by gneissic and granitic Palaeozoic basement rocks.





The southern limit of the basin is underlined by the regional Cévennes fault system that separates the Causses from the alpine domain (SE basin).



Geological cross-section along the Tournemire URL

The formation in which the tunnel was excavated is a fine-grained sedimentary rock composed predominantly of indurated clay particles, commonly referred to as argillites. The 250-metre thick argillaceous layer is surrounded by limestone rocks. It is 180 million years old and formed within a marine environment.

Usually less prone to fracturing than other types of rock (limestone and granite, etc.), the argillaceous rock at Tournemire nonetheless features some faults and fractures of various sizes (millimetric to decametric scales) that formed 40-50 million years ago (formation of the Pyrenees mountains) or issued from the reactivation of earlier structures (opening of the Tethys ocean, Middle Jurassic \approx 170 million years ago).

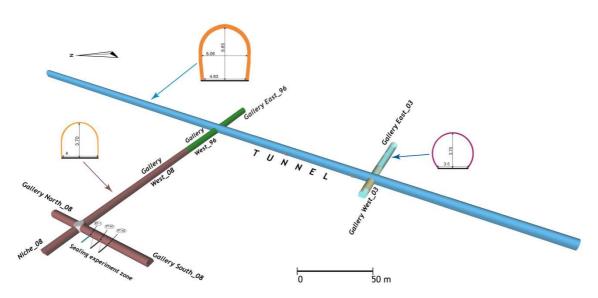
5.4.2.2 TOURNEMIRE TUNNEL AND THE EXPERIMENTAL STATION

Excavated at the end of the 19th century, the Tournemire railway tunnel is 1'885 metres long. It represents a unique opportunity, among other things, to observe the disturbances generated by an underground engineering structure excavated 120 years ago in an overconsolidated clay formation.

The experimental station itself is made up of the former railway tunnel, six drifts which have a total length of 285 metres and over 225 boreholes excavated since 1999.







General view of the Tournemire URL

5.4.2.3 MAIN EXPERIMENTAL PROGRAMS

A range of measuring equipment and observation techniques are deployed at the station to analyse the argillite and its behaviour, the principal experimental programs that have been developed at Tournemire are related to:

- Mechanisms responsible for the transfer of water and natural substances present in the clay formation;
- Effects of excavation and of using the underground engineering structures on the rock's containment properties;
- Faults and discontinuities detection techniques using a wide array of geophysical methods;
- Effects related to interaction between the rock and the exogenous materials, such as concrete and metal components;
- Performance of important components for the long-term safety of a geological repository, such as seals.

A brief overview of the R&D topics that has been addressed at Tournemire is summarized hereafter.

Migration of water in the argillaceous rock – Geochemical data

The argillaceous rock at Tournemire is composed of approximately 50% clay, the remaining portion being composed of quartz, carbonates, and secondary minerals (pyrite, etc.). Compact and hard, it contains very little water (3.5-4.5% in weight), which is trapped in pores around ten nanometres in diameter (porosity ranging between 7 to 8 %).

Apart from fractures, the rock studied at Tournemire exhibits an extremely low water permeability (< 10^{-14} m/s). The analysis of hydraulic tests and natural tracer profiles obtained for the whole argillaceous layer confirm that water circulates very slowly, about one centimetre per million years under the naturally imposed gradient. The major method of

SITEX





radionuclide transfer is therefore limited to the molecular diffusion process. However, through certain tectonic fractures and joints water may circulate more rapidly. Geochemical results indicate that water flowing within these fractures and joints originate from the calcareous formations located on either side of the clay layer and that they have a residence time of around 15,000 years. In comparison, water circulating through the calcareous rock on either side of the argillite layer has residence times of around 50 years.

Effects of excavating in the argillaceous rock – Geomechanical and Geophysical data

The mechanical properties of the argillaceous rock at Tournemire, and the fact that it is compact and hard, make it brittle. Excavation works therefore create mechanical disturbances extending from a few tens of centimetres (in the drifts) to around two metres (in the 120 year old tunnel), causing irreversible plastic deformations, manifested by the development of fractures. The extent and the intensity of this area, so-called the EDZ (Excavation Damaged Zone), evolve over time due to the different thermal, hydraulic and chemical loadings. More permeable than the undisturbed argillite layer, the EDZ is likely to be a preferential pathway for water flow and solutes migration.

In addition to the mechanical disturbance caused by excavation for the engineering structures, there is further fissuring induced by the drifts ventilation and the subsequent desiccation of the rock (hydro-mechanical coupling phenomena).

Characterising these fractures and fissures, and how they develop in space and time is therefore an essential part of assessing the safety of long-term disposal. In addition to classical methods (cores and boreholes survey), this has also been achieved using geophysical method (borehole seismic, multichannel analysis of surface waves, electrical resistivity 2D tomography).

Detection of tectonic faults (tectonic discontinuities) – Geophysical data

Due to the specific geological history of the Tournemire area, several families of faults occur in the argillite. Especially, strike-slip secondary faults (small vertical offset lower than 2 m, length on the order of hundreds of meters, thickness ranging from meter to tens of meters) are well evidenced by observation made from the underground drifts.

Detecting accurately such faults in clayey rocks from surface geophysical surveys and from existing underground drifts remains one major challenge, even using high resolution seismic surveys. Therefore, an important effort has been spent to pushing the methods as much as possible, including development of new interpretation methods, in order to evaluate the potentialities and limits of these geophysical methods.

Insights and conclusions gained in these research works have been used extensively for the technical expertise of the geological part of the implementer's dossier.

Disturbances to the rock associated with exogenous materials – Geochemical data

The purposes of these experimental programs were to identify and characterise the disturbances caused to the rock by materials brought into the geological environment from the outside. Dedicated experiments were thus conducted on cementitious (lime, concrete and hardened cement paste) and metal materials (iron) used in support lining or as plugs for closing the mouth of disposal cells. Interactions between these materials and the clayey





minerals in the rock can alter the geochemical properties of the rock and compromise its ability to contain radionuclides (swelling and containment properties alteration). The samples analysed from the chemically-disturbed zone reveal that alteration fronts can be as large as a few centimetres in the presence of water, and this over a period of contact ranging between one to a few decades.

The Tournemire experimental station is an exceptionally useful tool for this type of test: the lime used as cementing material for the facework masonry in the tunnel, which is similar to concrete, has been in contact with the rock for over 100 years, in other words, for a period comparable to the operating lifetime of a disposal facility.

Performance of disposal sealing components – Geomechanical data

The safety of a long-term geological disposal facility largely depends on the effectiveness of the systems used to close up the engineering structures. In particular, these systems imply the use of seals. These are made of a natural swelling clay-based material which ensures continuity of the containment provided by the rock.

At the Tournemire experimental station, the SEALEX research project is dedicated to assessing the effectiveness and robustness of such seals over time. This project involves examining the key factors that regulate the long-term hydraulic performance of the seals.

5.4.3 Ongoing and future R&D actions

The purpose of this chapter is to present a non-exhaustive list of the future R&D actions that will be performed at the Tournemire Experimental Platform during the next 5 years. The key issues and their associated experiments are addressed within the Tab. 2 below.





Tab. 2. Main ongoing experiments at the Tournemire URL

Key issues	R&D needs	Tournemire in situ experiment
Long-term stability: Performance assessment	 Perturbations and their influence on the confinement properties of the disposal components Technical feasibility of seals with respect to their safety functions and their expected performance level 	SEALEX SEALing EXperiment
Long-term stability: Internal perturbation	Engineered Barrier System / Host rock interactions in saturated conditions at 70°C - Chemical evolution (solid and pore solution) - Microstructure evolution - Composite effective diffusion coefficient evolutions - Validatation of numerical blind simulations	CEMTEX Cement Temperature EXperiment
	Estimating the duration of the oxidising transient within the steel/clay interfaces - Host rock oxygen consumption (with and without steel) at different humidity degrees	OXITRAN OXIdising TRANsient
Groundwater and radionuclide movement: Water flow in clay host	Water transport properties within a fault zone - In situ hydraulic testing - Mineralogical and petrophysical parameters - Porewater chemistry - Natural tracer profiles - Diffusion parameters (through and radial diffusion)	FRACTEX FRACture Transport EXperiment
rock	 Hydraulic behaviour of faults and fractures Porosity characterisation (nano- to microscopic scales) Mineralogical and chemical evolutions Magnetic properties 	PFAT PetroFabric analysis of the Toarcian Argillite of Tournemire





	Evaluating fault seal integrity - In situ characterisation of hydraulic, elastic and strength properties - Estimation of flow times and lengths within different fault zones - Permeability-stress-strain evolution of silty claystones and mudstones - Geophysical imaging the architecture of a fault zone in clay rich formations	Hydro-Mechanical Properties of a Fault Zone
Natural faults detection and GD monitoring	Detection of natural faults from: - the surface (very high resolution 3D seismic survey et very high resolution 2D electric resistivity profile), using advanced interpretation methods - existing drifts (very high resolution seismic at drift walls) - Feasibility test on large-scale tomography based on muons flux measurements	Geophysical Survey

The aims and the motivation of the above experiments at Tournemire are summarized hereafter.

5.4.3.1 SEALEX

As a part of the overall IRSN R&D programmes that provides the bases for scientific expertise on disposal safety, the SEALEX project was built with specific focus on sealing systems efficiency (cell seals, gallery seals, shaft seals). The main objectives of the SEALEX experiments are to:

- Test the long-term hydraulic performance of sealing systems (in normal conditions, i.e. non altered), for different core compositions (pure MX80, sand/MX80 mixtures) and conditionings (pre-compacted blocks or in situ compacted powder);
- Quantify the impact of intra core geometry —construction joints in the case of precompacted blocks— on the hydraulic properties of sealing systems;
- Quantify the effect of altered conditions —an incomplete saturation of the swelling clay or an incidental decrease of the swelling pressure caused by a failure of the concrete confining plugs— on its performance, which tests the concept robustness with respect to the hydraulic characteristics of the system.

The SEALEX project does not aim at demonstrating sealing capabilities of a geological disposal, which is the implementer's responsibility, but is devoted to test various technical parameters that could influence global hydraulic and mechanical performances of a seal. Furthermore, the SEALEX project will provide IRSN with feedback and knowledge on the key parameters that the implementer should specify and control in situ.





5.4.3.2 CEMTEX

The topic of clay/concrete interactions has been widely studied in the literature. Though a large amount of studies have been conducted on clay and/or clayey rock geochemical evolutions in an alkaline environment, very little is known on the cementitious material evolution.

During the last decade, the few studies that were performed on representative interfaces between cementitious and clayey materials (laboratory or under in situ conditions) were carried out at temperatures ranging from 15 to 50°C. However, is now generally accepted that the temperature in the future HLLW geological disposal site will reach at least 70°C and will hence modify more significantly the reactive mechanisms and potentially accelerate the extension of the perturbation front in both materials.

For this reason, IRSN has just started a new R&D project called CEMTEX which main objectives are to:

- Create cementitious material/argillite interface in saturated conditions at 70°C to characterize accurately: 1/ the chemical evolutions of the cementitious and clayey materials; 2/ the evolution of the porosities; 3/ evolutions of the composite hydrodynamic properties;
- Cross-characterizations results between *in situ* and laboratory experiments to estimate the length scale influence;
- Validate blind numerical simulations (water/rock equilibrium in concrete and clays + reactive transport at the interface) at 70°C.

5.4.3.3 OXITRAN

The geological disposal for high level waste (HLW) involves stainless and carbon steel components. Up to now, most studies on steel corrosion in clayey media have been focused on reactivity under reducing conditions since, at the timescale of the geological disposal, minerals such as pyrite are supposed to impose a reducing environment. However, soon after closure of HLW cells, the entrapped oxygen introduced in the disposal cell during the operational stage may induce an oxic corrosion of metallic structures until the whole consumption of oxygen. Under humid conditions, oxic corrosion may lead to drastic corrosion rates. Therefore, the assessment of steel corrosion can crucially depend on the oxidizing period and its duration

The OXITRAN (OXIdising TRANsient) project has been developed by IRSN to understand the evolution and the duration of the oxidizing transient in the Tournemire argillite, in presence and absence of steel, and in unsaturated *in situ* conditions. This project aims at answering two questions:

- What is the oxygen consumption rate by the argillaceous rock for a given volume of gas and exposed rock surface?
- What is the oxygen consumption rate by steel corrosion for a given exposed metal surface, exposed rock surface and gas volume?

The main objective of such an experiment is finally to build a sufficient knowledge on oxygen

SITEX





consumption in the conditions prevailing in a HLW disposal cell in order to model accurately the oxidizing transient and to transpose to long term simulation on disposal cells.

5.4.3.4 FRACTEX

The purpose of the FRACTEX project is to assess transport properties within fractures and faults through a series of *in situ* and laboratory experiments. The different tests aim at evaluating the contribution of both diffusive and advective processes on water flux through a (1) damaged (2) disturbed and (3) undisturbed argillite rock.

The targeted structure for this study is a narrow subvertical strike-slip fault zone displaying a 2 meter vertical offset. A 50 meter-long horizontal borehole (diameter 101 mm) will intercept the structure at a distance far enough from the tunnel and drifts so as to minimize the hydro-mechanical perturbations of the excavation damaged zone (EDZ). Mineralogical and petrophysical characterization of the rock will systematically be performed along the entire borehole.

Immediately after drilling, the borehole will be equipped with a Mini Multiple Packer System (MMPS) where *in situ* hydraulic tests (pulse-test) will be performed on the damaged, disturbed and undisturbed argillite rock. Additional laboratory hydraulic tests will be carried out on argillite samples selected to represent the different rock conditions (damaged, disturbed and undisturbed argillite).

To complete this hydraulic characterization, radial and through diffusion experiments of artificial water (HTO), anionic ($^{36}CI^{-}$) and cationic ($^{22}Na^{+}$) radiotracers are also planned. The comparison between the time required to propagate a perturbation by advection and the diffusive transport time will allow to assess the relative significance of advective and diffusive transport for the different rock conditions.

The FRACTEX experiment will also give the opportunity to acquire a horizontal profile of natural tracers (2 H, 18 O, Cl⁻) and noble gas (4 He) distribution in the pore water. The data will be obtained by means of equilibration methods (vapour-exchange and radial diffusion experiments).

5.4.3.5 PFAT

This project aims at investigating the petrofabric (porosity, mineralogy and textural organization) of a fault zone from the Upper Toarcian argillites of Tournemire at different scales (millimetric to nanometric) by XRD, TEM, SEM-EDS, X-ray microtomography and Focussed Ion Beam (FIB) methods.

This study will focus on characterising the (1) undisturbed and (2) disturbed argillite, and in particular the dark bands within one of the Tournemire fault zones that is interpreted as resulting from a phenomenon of called "clay smearing" (often suggested as fault sealing mechanism). The results will enable significant improvement in characterizing mineralogical and permeability modifications within a clay-based fault zone and could explain the hydraulic behaviour of a sealed fault (FRACTEX).





5.4.3.6 HYDRO-MECHANICAL PROPERTIES OF A FAULT ZONE

The objective of this project is to define a permeability-stress-fluid pressure law from a sealed fault zone at the Tournemire Experimental Platform based primarily on parameters measured from in situ experiments.

Two main questions will be addressed through this project:

- At what overpressure will the permeability of a clay-based fault increase for a given stress condition and tectonic context?
- In a defined condition and for a given overpressure, which mechanical conditions will cause significant permeability increase?

In order to answer these questions the project is organized in three tasks: field experiment, laboratory experiment and modeling.

- Task 1 is a mesoscale experiment, the aim is to perform in situ permeability test in a fault zone while monitoring strain and microseismicity.
- Task 2 is a series of laboratory experiments which aims to characterize the evolution of Vp, Vs and permeability during deformation in the laboratory of the material from the mesoscale experimental site.
- Task 3 is the numerical modeling. The primary objective of the modeling is to test the proposed permeability-stress-pore pressure on the experimental results (both mesoscale and laboratory scale). Classical continuum mechanics approaches (Finite Element and Finite Difference Methods) will be used to assess effective properties from the mesoscale experiment. Discrete Elements (DEM), will be used to address coupled deformation processes at the micro-scale, and to provide insight on laboratory to formation scale change.

5.4.3.7 GEOPHYSICAL SURVEY

Advanced evaluation of detection methods for natural discontinuities from the surface, using very high resolution surveys (3D for seismic, 2D for electrical resistivity), coupled with innovative treatment methodologies (e.g. non local method based on Common Reflector Surfaces, and modeling).

From the existing undergrounds drifts, application of seismic methods (reflection, transmission, guided waves), survey of the background acoustic noise.

Last, a feasibility test is foreseen to test the potentialities (and difficulties) of a large-scale tomography based on muons flux measurements, which is believed to provide valuable information to follow the geological disposal evolution in time.

5.5 GERMANY

The competence fields "Waste Disposal", "Assessment of Long-term Safety", "Geochemical Research", "Research in Underground Laboratories" and "Geochemical and Geotechnical Laboratory" are mainly oriented towards safety analyses and geosciences. Priority is given to the development of methods and instruments for the performance of safety analyses and experimental research on the examination of waste disposal concepts and the provision of data and models that are relevant with regard to safety in the long term.





5.5.1 Geoscientific Laboratory

The Brunswick location of GRS maintains a geoscientific laboratory. In this laboratory geochemical and geotechnical issues with regard to the underground disposal of radioactive and hazardous chemical waste are investigated. The laboratory represents a unique position within GRS, as it is the only field of activity in which experimental basic research is practised.

Research topics

The geoscientific lab deals with various tasks about environmental research and repository safety research. The research and development (R&D) tasks comprise of, amongst others, the investigation of geological rock formations as well as radioactive and hazardous chemical wastes. Some relevant issues relates to the properties that a respective rock formation has to provide for waste disposal and what are the advantages and disadvantages of final waste disposal in salt rock, clay or granite.

Other issues comprise the mobilization and release behaviour of contaminants, the overall properties of the above-lying rock strata, the effects of technical barriers and, in addition, their interactions with each other.

Areas of focus

The following methods are applied when carrying out experiments and analyses relating to these issues:

1. Geochemical investigations are dedicated to the properties, behaviour and interaction of the different host rock types, the overlaying rock strata, waste, technical barriers and any possible inflowing saline water. The host rocks: salt rock, clay and granite are, for example, due to their geological history composed differently and therefore, have different properties.

2. Geotechnical investigations allows as an example the investigation of the permeability of a rock with regards to gases and water or the technical barrier under the influence of heat or pressure. This, in turn, allows for example the simulation of natural conditions or the special conditions of a repository.

3. The extraction, preparation and transport of samples, for example of saline solution from a salt mine, need a lot of expertise and state-of-the-art equipment. This is due to the fact that the results will only be considered both credible and valid if the samples have been extracted properly and during the transportation to the analysis in the laboratory remain unchanged.

Depending on the specific questions and research methods, the work will be performed besides in the laboratory itself also in a technical centre (for larger investigations for example, on boulders or slabs of rock) or in situ i.e. at a mine or in an underground research laboratory.





5.5.2 Underground Laboratory

In former times the Asse salt mine was used as a disposal facility for low and intermediate level waste and as an underground research laboratory. Especially disposal techniques in salt were developed from 1965 to 1995. These techniques included also demonstration tests for the direct disposal of spent fuel e. g. the thermal simulation of drift emplacement, heating tests, construction of a dam and emplacement methods.

Currently the Asse mine is in a decommissioning state.

Some tests and investigations in salt are performed also in the salt mines Bernburg and Salzdetfurth. Furthermore, GRS participates in several international projects in underground laboratories e.g.

- international research in clay (Mont Terri Switzerland)
- in-situ investigation (Bure France)
- international research in granite (Äspö Sweden)

5.6 LITHUANIA

There is no experimental installation like underground research laboratory in Lithuania. There is no experimental laboratory in LEI for the research on issues related to radioactive waste disposal. Currently there are no plans to establish such facilities in LEI, the experimental research on particular issues like geotechnical and geochemical characteristics of the host rock might be carried out in other certified laboratories in Lithuania.

5.7 NETHERLANDS

The Dutch concept for a Deep Geological Repository (DGR) for disposal of radioactive waste is still being developed. Since the Dutch radioactive waste will be stored in dedicated surface facilities for a period of at least 100 years the determination of a suitable concept is at present not a critical issue. In the past, attention mainly has been focused on suitable salt domes in the northern part of the Netherlands. At present research efforts are now carried out in the framework of the five-year program OPERA¹, in which the focus is mainly on Boom Clay as host rock.

The Netherlands does not operate an underground research laboratory, and NRG has no specialized experimental facilities in the Netherlands dedicated to deep geological disposal. There are however some experimental research efforts performed at several Dutch institutes and laboratories in the framework of the OPERA program. These efforts are summarized below.

5.7.1 Lithological characterization of Boom Clay

The geohydrological, geochemical and geomechanical properties of sediments are strongly dependent on the lithology. The up-scaling of Boom Clay properties measured on the lab

¹ OPFRA is the Dutch acronym for research programme into geological disposal of radioactive waste





scale to a regional scale therefore require a proper insight on the lithological variation on the various scales.

As part of the OPERA program, the present regional lithological variation of the Boom Clay in the Netherlands will be characterized based on a petrophysical evaluation of well logs of a sub set of key Boom Clay intervals, in conjunction with the grain-size analysis results from 50 wells, spread across the Netherlands. Both the vertical and lateral trends in heterogeneity will be assessed, using the statistical characteristics of the measured data. These statistics will also be used in an uncertainty analysis. Together with existing sedimentological knowledge of the Boom clay, this will lead to an enhanced conceptual lithofacies model of the Boom clay, which will be used in the subsequent geohydrological characterization activity (see next section). Towards the concluding stage of this activity the focus will lie on the areas where the Boom clay is present at depths > 400 m and has a thickness >100 m.

5.7.2 Geohydrological characterization of Boom Clay

The Netherlands Organisation for Applied Scientific Research (TNO) and NRG will combine existing lab and in situ porosity and permeability measurements of the Boom Clay with the updated lithological and lithofacial concepts to derive a regional scale concept of present porosity lateral and vertical permeability distributions within the Boom Clay in the Netherlands, including an estimation of the uncertainty range.

5.7.3 Geochemistry and geomechanics of Boom Clay

A consortium led by the Netherlands Organisation for Applied Scientific Research (TNO) performs research to gain insight into the geochemical properties of the Boom Clay in order to establish the reactivity towards radioisotopes, the physical properties that depend on sediment-geochemical characteristics, and the evolution of the Boom Clay at the geological time scale. The associated aims of these activities are: (1) to establish analytical data on the geochemical properties of the Boom Clay at a national scale, (2) to characterise the reactivity of the Boom Clay, (3) to characterise pore water in the Boom Clay and groundwater in adjacent aquifer layers and (4) to set-up a prognosis on the long-term geochemical properties of the Boom Clay under anticipated future geological evolution of the Netherlands.

The experimental research efforts consist of a series of standard analyses on Dutch archive samples from the Boom Clay, standard and non-standard analyses on newly collected samples, sampling of wells having screens just above or below the Boom Clay, and extracting pore water from fresh Boom Clay sediment samples. Fresh samples will be taken from new drillings into the Boom Clay, or otherwise samples will be collected in Belgium from quarries and the underground laboratory in Mol (HADES).

The results of this project will primarily lead to a database consisting of national, statistical data about the geochemical properties of the Boom Clay in the Netherlands and the groundwater above and below this geological layer including insight into their lateral and vertical variability. Additionally, detailed insight into the redox and sorption properties will be delivered when new drillings will be performed.





5.7.4 Migration of radionuclides through Boom Clay

Within the OPERA program, the University of Utrecht carries out experimental research on the effects of redox properties of Boom Clay on radionuclide sorption and speciation. Redoxactive constituents of Boom Clay will be identified, the redox state of the Boom Clay matrix will be determined, and its electron donor and acceptor properties will be characterized. Part of the characterization will be achieved using state of the art electrochemical techniques. In addition, the relationship between the redox properties of Boom Clay and the redox speciation of selenium (Se) and uranium (U) will be determined, and the consequences of Se and U reduction on the sorption or/and solubility of these elements will be investigated. This will include the characterization of Se and U reduction products in Boom Clay with sophisticated techniques (stable isotope analyses, X-ray analyses, Laser Ablation ICP-MS).

5.7.5 Monitoring

A topic that is treated outside the OPERA program, but which is considered essential in the Netherlands is monitoring. The Dutch licensing system requires monitoring of radiological conditions, the state of the waste (containment) and discharges from facilities, such as radioactive waste treatment plants and stores. This requirement is especially important in relation to phased disposal concepts in which waste retrieval is explicitly accounted for.

NRG participates in the EU FP7 project MoDeRn² which aims to provide an understanding of monitoring activities and available technologies that can be implemented in a deep geological repository, and to provide recommendations for related, future stakeholder engagement activities. NRG focuses for an important part on the further development and implementation of wireless, through-the-earth monitoring and data transfer techniques, including modulation/demodulation techniques and signal analysis. The research efforts are partly carried out at the HADES³ URL (Mol, Belgium) in cooperation with ESV Euridice, the operator of the facility.

5.8 SLOVAKIA

There is no experimental installation like underground research laboratory in Slovakia, neither experimental laboratory in DECOM for the research on issues related to radioactive waste disposal.

However, above ground laboratory experiments have been successfully conducted by Slovak University of Technology and State Geological Institute of Dionýz Štúr.

SITEX

² Monitoring Developments for Safe Repository Operation and Staged Closure; http://www.modern-fp7.eu/ <u>³ HADES: High Activity Disposal Experimental Site</u>





5.8.1 Slovak University of Technology

Laboratory investigation was aimed at comparison different methods of hydraulic conductivity determination for 105 clay samples from different localities in Slovakia. Hydraulic conductivity was determined in a triaxial cell apparatus by Constant head permeability test, measuring the flow of water through the sample. The triaxial test determination with a pore pressure apparatus gives substantial control over the hydraulic gradient across the sample. Magnitude of the gradient was in the range 30 to 100. Laboratory investigations of consolidation of soils in oedometer were performed to determine coefficient of consolidation by oedometer Taylor's method and to calculate the hydraulic conductivity.

5.8.2 State Geological Institute of Dionýz Štúr

The experimental research on particular issues like geotechnical characteristics of the host rock might be carried out in Laboratory of engineering geology SGIDS. Besides common laboratory test few special test methods could be provided; Technique of squeezing of pore water from the rock samples (in cooperation with Laboratory of engineering geology at the Department of engineering geology, Faculty of Natural Sciences, Comenius University) with following isotope analyses. The triaxial chamber, suitable for testing of very low permeable soils could be used for Percolation test, which is basically the permeability test in triaxial apparatus with collecting of percolated water for following analyses of the water to observe the water content differences in time.

5.9 SUMMARY

The summary of laboratory facilities and installation, studying specific issues, available for each beneficiary, is listed in Tab. 3. The overall summary of scientific and research labs and installations is listed in Tab. 4.





Tab. 3. Summary of laboratories and installation, studying specific issues, available for SITEX beneficiary for potential R&D actions

Installation for specific issue/ Beneficiary	Radiation issues (Waste, canister)	Geomechanical issues (EBS, host rock)	Geochemical issues (interaction, migration, host rock, EBS)	Geology, hydrogeology
BEL V FANC	No	No	Cooperation (IRSN, Universities)	No
CNSC	No	Cooperation	No	Cooperation
UJV Rez, a.s.	Yes	Yes (limited)	Yes	Yes, cooperation
IRSN	Yes	Yes	Yes	Yes
GRS	No	Yes	Yes	Yes
NRG/ELI	Hot Cell Lab (NRG)	Cooperation (TNO)	Cooperation (Uni Utrecht)	Cooperation (TNO)
LEI	No	Heat transfer laboratory	No	Cooperation
DECOM	Cooperation (VUJE – waste)	Coop (GUDS, Tech. University)	Cooperation (GUDS, Tech. University)	Cooperation (GUDS, Tech. University)





Tab. 4. Summary of scientific installation, available for SITEX beneficiary for potential R&D actions

Beneficiary	Labs	Coop/ subcontracting	URL/ cooperation in URL	Monitoring (which kind)	Plans
BELV FANC	No	Yes	No, coop in Mont Terii		??
CNSC	No	IRSN, universities	No, coop with IRSN	Radionuclides in soil and water	Cooperation with university, Decovalex
UJV Rez, a.s.	UJV (radiochemistry, migration properties, buffer+backfilil properties, package properties	Universities, research institutions	No, coop in GTS and Josef gallery	GW properties Radionuclides in soil, water and air	Lab for mid- scale Anaerobic lab
IRSN	LAME (physical, radiological, and chemical characterizations of soils, rocks, and waters)	Geomechanics	Yes, Tournemire Cooperation in Mt. Terri	Geomechanical properties GW properties System parameter evolution (T, seatide,) Radionuclide monitoring (Rn)	Experiments in Tournemire
GRS	Geoscientific lab (geochemical and geotechnical issues)	Universities, research centres	Yes (salt mine). Cooperation in Mt. Terri, Bure, GTS	Environmental monitoring (soil, water, air)	International cooperation
LEI	Installation for heat transfer	No	No	Currently not	Will depend on national programme to be developed till August 2014

SITEX



Sustainable network of Independent Technical Expertise for Radioactive Waste Disposal



NRG/ELI	Hot Cell Lab and actinide lab (NRG)	Yes (TNO, Uni Utrecht, GRS)	No, coop with HADES	Cooperation with foreign URLs; in situ demonstration of innovative monitoring techniques	WIPP URL can be an alternative
DECOM	No	Yes (GUDS, TechUni)	No	Cooperation (VUJE): Radionuclides in soil and air	-

6 Modelling capacities

6.1 BELGIUM

Bel V conducts independent modelling investigations in order to assess the safety assessments provided by operators for radioactive waste repositories. The main objectives of these independent modelling activities are to improve the Bel V understanding of the modelling approach followed by the operator (e.g. the conceptual model, the main hypotheses, the calculation code), to identify potential difficulties/weaknesses, to verify the appropriateness of input parameters, to challenge safety margins by performing sensitivity and uncertainty analyses and to test model capabilities (e.g. by using multiple models or codes).

This section first describes Bel V computational resources (section 6.1.1) and the current modelling capabilities of Bel V (section 6.1.2) in order to support the review of safety assessments for radioactive waste repositories. Finally, section 6.1.3 describes the topics in which Bel V plans to further develop its modelling capabilities.

6.1.1 Computational resources

Bel V has a computing server dedicated to its R&D projects requiring significant computational resources. Bel V has equally several recent PCs for performing calculations which require only limited computational resources.

6.1.2 Modelling expertise

In order to support the review of safety cases for radioactive waste disposal facilities, Bel V has principally developed modelling capabilities in order to verify assumptions made by operators in models devoted to (i) the migration of radionuclides in the near and far-fields of waste disposal facilities, (ii) the geochemical evolution of engineered barriers, as well as to (iii) radiation protection. More information about Bel V capabilities in these three main





topics is provided in the following sections.

Topic 1: Radionuclide migration

Bel V progressively develops modelling capabilities in independently verifying assumptions made by operators in models devoted to the migration of radionuclides into radioactive waste disposal systems (near-surface and geological repositories). The advective and diffusive transport of radionuclides in the near- and far-fields of radioactive waste repositories is modelled by Bel V under saturated and unsaturated conditions, with one or two-dimensional models. These models are developed by Bel V with the commercially available HYDRUS 1D and HYDRUS 2D STANDARD software packages⁴, as well as with the MELODIE code⁵ developed by the IRSN specifically for the regulatory review of safety assessments for radioactive waste disposal facilities.

Whereas Bel V does not develop its own codes for assessing the safety of radioactive waste disposal facilities, it regularly develops computational routines to allow performing batch calculations, the post-processing of modelling results and sensitivity analyses (for instance Monte-Carlo analyses).

Finally, Bel V has participated in the previous 6FP EC projects PAMINA and MICADO. Within the framework of these projects, Bel V has developed capabilities in the following fields:

- Sensitivity analyses (6FP EC PAMINA). Bel V has notably highlighted that the sensitivity of Safety Assessment to the Probability Density Functions associated with input parameters is high. The study stressed that a conservative assumption for PDFs is not possible in general without a dedicated study and detailed justifications.
- Modelling of the radionuclide release from waste packages and spent fuel (6FP EC MICADO). This modelling is of particular concern as it has a deep impact on the long term safety of radioactive waste disposal. As highlighted by the 6FP EC MICADO project in which Bel V participated, the modelling of the spent fuel Instant Release Fraction (IRF) is an important point of attention.

Topic 2: Geochemistry

Bel V progressively develops modelling capabilities in verifying assumptions made by operators in models devoted to the geochemical evolution of confinement barriers of a waste disposal system. Bel V uses the PHREEQC software that allows performing speciation calculations, involving chemical reactions between chemical species in minerals, aqueous and solid solutions, as well as in gaseous mixtures.

Topic 3: Radiation protection

Bel V has develops modelling capabilities in verifying assumptions made by operators in models devoted to radiation protection. Bel V particularly uses the MCNPX software to evaluate the radiation protection aspects of specific situations.

 ⁴ HYDRUS 1D and 2D STANDARD are developed by « PC-progress ». See <u>http://www.pc-progress.com</u>.
 ⁵ The use of MELODIE by Bel V is allowed by a collaboration agreement between Bel V and IRSN.





6.1.3 Further development

This section summarizes the topics in which Bel V plans to further develop its modelling capabilities and the corresponding R&D actions that may be undertaken.

Topics to further investigate

The codes used by Bel V to model radionuclide migration in radioactive waste disposal systems (HYDRUS 1D, HYDRUS 2D STANDARD and MELODIE) are developed for the modelling of non-reactive transport phenomena. Consequently, these codes are unable to model the geochemical evolution of the confinement barriers due to chemical reactions between the barrier materials and the pore water. As the geochemical composition of the confinement barriers will influence radionuclide transport parameters (e.g. barrier porosity, sorption capacity ...), a coupling between the modelling of the radionuclide transport and the concurrent geochemical evolution of the confinement barriers should be performed.

Bel V plans to progressively develop capabilities in modelling reactive transport phenomena using chemical-coupled transport codes. Such models may be developed with simulation platforms such as HYTEC⁶.

Up to now, the R&D programme of Bel V devoted to radioactive waste disposal facilities has mainly focused on modelling the migration of radionuclides in the near and far-fields of repositories. Bel V plans to progressively strengthen its modelling capabilities in verifying assumptions made by operators in models devoted to site hydrology and biosphere.

Main type of actions

Bel V may develop capabilities in the above mentioned topics by undertaking three main types of R&D needs for knowledge (see section 5.1 of deliverable 3.1 [1]):

- A. Literature survey, participation to conferences or international working groups (IAEA, OECD);
- B. Sub-contract to other organisations (universities and research centres);
- C. R&D within Bel V or in collaboration with other organisations (FANC, ETSON, Framework Programmes of EC,...).

The choice of the action type is dictated by the importance and priority of the issue and by the availability of resources and competences within the regulatory body (FANC and Bel V).

6.2 CANADA

6.2.1 Modelling capacities in geosciences

CNSC has a long-standing modelling capability in geomechanics. CNSC has the code of COMSOL and its supporting modules that can be used for the modelling of the geomechanical and external disturbance issues. The modelling that has been done includes the numerical modelling of the excavation damaged zone (THM process), glaciation (past and future) effects, and gas migration through developing conceptual and mathematical

⁶ HYTEC is developed by « Ecole des Mines de Paris ». See <u>http://hr.geosciences.ensmp.fr/modelisation/hytec.</u> SITEX





models. CNSC will maintain this modelling capacity for the future R&D actions that are needed for the management of nuclear wastes.

CNSC has also maintained capability and obtained the codes of Modflow and Cormix for groundwater flow modelling and mixing zone modelling to support the environmental impact assessment. In addition, CNSC has identified some other important R&D issues such as corrosion of waste containers and long term performance of seals that will need further R&D actions. CNSC might consider enhancing/developing its modelling capability in these areas.

6.3 CZECH REPUBLIC

A number of computers codes are available in UJV for predicting evolution and safety of repository:

- 1) Inventory of spent fuel assemblies and structure materials (MCNP–a general Monte Carlo n-particle transport code (SCALE. A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, ORIGEN 2.2).
- 2) Criticality of waste packages under various conditions (MCNP–a general Monte Carlo n-particle transport code).
- 3) Thermal evolution of repository (TOUGH2).
- 4) Gas transport in repository (TOUGH2)
- 5) Geochemical speciation codes (PHREEQE, Geochemical Workbench, TOUGHREACT).
- 6) Hydrogeological codes (FEFLOW, TOUGH2).
- 7) Integrated computer codes for predicting possible effective doses from repositories (GoldSim, PAGODA, Amber, RESRAD).

The modelling group consists in two modellers with good knowledge of integrated codes such as GoldSim, which is used as a standard model for conduction safety analyses. The modellers are supported by specialists who provide for safety case the hydrogeological, geochemical data and other data using process computer codes such as FEFLOW or PHREEQE.

6.4 FRANCE

IRSN has developed during the last 10 years many nuclear safety and radiological protection computer codes and is involved in several consortiums for the development of modelling tools related to deep geological disposals. IRSN also uses when needed either commercial or academic codes whenever required.

6.4.1 Radionuclide migration

6.4.1.1 MELODIE (MODEL FOR LONG-TERM ASSESSMENT OF RADIOACTIVE WASTE REPOSITORIES)

The MELODIE software program is IRSN's reference tool for assessing the impact of a deep geological repository on the geosphere by calculating the transfer of radionuclides through a





porous and fractured medium. This software is designed to model a disposal site factoring in all the main physical and chemical characteristics. These are represented in simplified form, adapted to large scales of time and space required for simulation.

The computational code models water flow and the phenomena involved in the transport of pollutants in porous media in 3 dimensions -or in 2 dimensions using vertical sections; physical and chemical interactions are represented by a retardation coefficient integrated in the computation equations. These equations are discretised thanks to a method called the FVFE method - "Finite Volume Finite Element" -, which is based on a Galerkin method to discretise time and variables, together with a finite volume method using the Godunov scheme for the convection term. The FVFE method is used to convert partial differential equations into a finite number of algebraic equations that match the number of nodes in the mesh used to model the site assessed. It also serves to stabilise the numerical scheme. The conjugate gradient method is used to solve the system of equations.

MELODIE has been used many national and international projects, such as the NF-Pro Project (an FP6 project) relative to understanding and modelling the physical and chemical parameters found in deep geological repositories. In this case, the transfer of different radionuclides was computed using a model made up of different meshes combined together. This made it possible to simulate the behaviour of a disposal facility, from near field – including the factors of engineered barriers and package decay kinetics – to far field – including the characteristics of the host rock. The method uses PVM software to transfer the boundary conditions to the various meshes.

6.4.1.2 DIPHPOM (DIPHASIC WATER-GAS MIGRATION IN POROUS MEDIA)

In collaboration with University of Claude Bernard in Lyon, IRSN is developing DIPHPOM, a 3D simulation tool to simulate water-gas migration in porous media. It takes into account the convective and diffusive transport of N components in 2 phases as well as mass exchanges between phases (dissolution and evaporation). The liquid phase and the solid matrix are assumed incompressible (except that porosity can become a function of fluids pressure); the gas phase follows the ideal gas law. The formulation is based on the classical mass conservation laws for both multi-component phases (g for gas and I for liquid) supplemented with generalized Darcy equations for each phase. These equations are completed by an appropriate set of closure equations related to the hypothesis of the existence of a local thermodynamical equilibrium (Henry law, Raoult-Kelvin law...). In order to handle material heterogeneities as well as changes in the thermodynamical state of the system (one or two phases present), a special set of unknowns is chosen, namely liquid pressure PI and molar fraction of dissolved gas (for example hydrogen) Xli. The resulting system of non-linear equations is treated with fully implicit time discretization and with an exact Newton method to obtain a set of linear equations. The spatial discretization has been done for triangles and tetrahedral elements with a finite element scheme. The implementation of Discontinuous Galerkin method is currently ongoing.

6.4.2 Geochemistry and reactive transport





6.4.2.1 PHREEQC

PHREEQC is a freeware computer code designed to perform a wide variety of lowtemperature aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations; (2) batch-reaction and one-dimensional (1D) transport calculations involving reversible reactions, which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibrium, and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes; and (3) inverse modelling, which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits.

IRSN has used the PHREEQC code to model:

- The thermodynamic properties of pore waters with dissolved H₂ (in unsaturated clays);
- The diffusion processes of an alkaline plume in a clay barrier.

6.4.2.2 HYTEC

HYTEC is a modular and upgradeable simulation platform, mainly composed of a hydrodynamic module (R2D2), a reaction module (CHESS) and a coupler. The approach is easily upgradeable and coupling with other modules is currently being considered (a module of river flow, for example).

The R2D2 module describes the flow of liquid phases (saturated flows, unsaturated flows, and transitory steady flows), the transport of heat and that of elements in porous or fractured environments in one, two or three dimensions. In view of the coupling, a scheme of finite volume spatial discretisation has been chosen. This scheme is particularly well suited to reactive systems. The flexibility of a Voronoï-type gridding used by default by R2D2 allows irregular domains, possibly very complex domains, to be meshed.

The CHESS module simulates the chemical reactions within each mesh of the model. CHESS is based on a powerful solution motor, highly optimized for coupled calculations. Chemical calculations use an extended thermodynamic database, allowing calculations to be performed at the equilibrium state. In addition, CHESS has a generalized kinetic approach, applicable to all types of reaction.

The HYTEC application fields range from simple systems of laboratory columns to integrated simulations of all the engineered barriers of a radioactive waste storage. It is applied to safety studies of gas geological storage, including the durability of wellhead concrete. As for emerging application fields, HYTEC is particularly well suited to the topic of solidified waste leaching and material biodegradation.

IRSN has used in recent years the HYTEC code to investigate:

- The near field evolution for deep a clay-based underground radioactive waste disposal;
- The physico-chemical evolution of clay/cement paste interface (simulation of the perturbation fronts extensions in both materials and to reproduce the evolution of

SITEX





chemistry, microstructure, mineralogy and hydrodynamic properties);

- The physico-chemical evolution of iron/clay interactions (mineralogical and transport evolutions) for HLW waste cells;
- Gas diffusion transport in the EDZ.

6.4.3 Hydrogeology

6.4.3.1 NSIGHTS: A NUMERICAL HYDRAULIC TEST SIMULATOR

nSIGHTS (n-dimensional Statistical Inverse Graphical Hydraulic Test Simulator) is a Windowsbased numerical hydraulic-test simulator that provides state-of-the-art well-test analysis tools for analysis of single-phase water and gas tests.

IRSN is now using nSIGHTS to estimate the permeability distributions within the Tournemire argillite rock from pressure pulse testing.

6.4.4 Geomechanics (multi-physics)

Two finite elements codes are currently mostly used in IRSN to solve geomechanical problems, either applied to simulating of field data obtained from experiments carried out in the Tournemire URL or in other URLS, or in surface laboratories.

6.4.4.1 CASTEM: A FINITE ELEMENT CODE FOR THERMO-HYDRO-MECHANICAL SIMULATIONS

Cast3M is a computer code developed by the French Atomic Energy Commission (CEA) for the analysis of structures by the finite element method. It is a powerful, flexible analysis and optimization program for solving mechanical linear elastic problem in statics and dynamics (vibration, extraction of eigenvalue), thermal and heat transfer problem, nonlinear problem (elastic, plastic, creep materials), step by step dynamic problem, etc. Cast3M includes a set of elementary processes (library of operators) that the user can bind to define and solve his problems.

6.4.4.2 LAGAMINE: A FINITE ELEMENT CODE FOR THERMO-HYDRO-MECHANICAL SIMULATIONS

LAGAMINE is an academic general purpose 2D-3D finite element code developed since the eighties at Liège University (Belgium). It can solve several types of boundary values problems: thermal (Fourier conduction, radiation), hydraulic (saturated and unsaturated Darcy flow, Fick diffusion) and mechanical (elasticity, plasticity, viscoplasticity, contacts with large displacements). The solution can be achieved either for uncoupled problems or for fully coupled solutions (e.g. Thermo-Hydro-Mechanical).

6.4.5 Other codes

IRSN has developed numerous other codes for its needs in nuclear safety or radiation protection for human health and environment such as:

• SYMBIOSE simulates the impact on human beings from a radioactive environmental contamination: it models the transport and transfer of radiation sources to the various environmental compartments, leading to a calculation of the dose received





by humans;

- AQUAREJ calculates the dose impact of radioactive discharges in rivers, associated with regular working of nuclear facilities;
- FOCON 96 estimates the dosimetric impact of atmospheric releases of nuclear installations during normal operation;
- ISIS is a computer tool dedicated to the study and the numerical simulation of fires in industrial facilities.

6.5 GERMANY

The simulation and modelling of processes relevant to deep geological disposal systems requires a broad range of numerical tools. Several thermal, mechanical, hydraulic and chemical processes and their interactions have to be considered which calls for sophisticated software that is capable to simulate coupled processes.

Codes for the simulation of flow and transport processes

Codes for the simulation of flow and transport processes are designed to meet specific requirements. Performance assessment models which consider the evolution of the entire repository system or are suitable for probabilistic analysis have to speed up calculation time by simplifying certain aspects e.g. by using networks of 1-dimensional grid structures or by neglecting certain processes. Process models, on the other hand, allow an in-depth analysis of specific problems but are not able to cover the whole range of relevant processes, components or time frames.

TOUGH2

The code TOUGH2 (Transport of Unsaturated Groundwater and Heat) was developed by Lawrence Berkeley Laboratory, USA, for the simulation of 3-dimensional multi-phase, heat and radio nuclide transport in porous media. A generalized Darcy-law is used to simulate density driven flow. By means of a set of alternative equation-of-state (EOS) modules different processes can be simulated. Saline ground waters e.g. can be treated with the EOS modules EOS7 and EOS7r.

Since 1991 GRS uses codes of the TOUGH2 code family to investigate processes in geological disposal systems. GRS has introduced several code modifications for processes which are relevant to such systems and are not covered by the standard TOUGH2 code. The modifications cover non-linear, salinity-dependent sorption, time-dependent boundary conditions, and pore compaction due to convergence of salt rock cavities. Code development continues.

In order to simulate thermal-hydro-mechanical interactions and gas migration processes in clay formations the code TOUGH2 was coupled to the geo-mechanical code FLAC3D by GRS in order to simulate three-dimensional, coupled thermal-hydro-mechanical interactions. In another branch of the code the mechanism of micro-crack dilation, which may significantly affect the migration of gas in argillaceous host rock and the pressure evolution inside the repository, was introduced.





The possibility to adapt the source code of TOUGH2 according to the current needs is a strong advantage of the software. In the review of the safety case of an applicant it gives the regulator the needed flexibility to investigate alternative physical processes and models. In principle, multi-purpose codes offer a similar flexibility, but the experience shows that indepth knowledge of a source code and self-contained code development fosters the required in-depth understanding of processes and numerical aspects.

<u>MARNIE</u>

The code MARNIE is an in-house development of GRS designed for the simulation of fluid and tracer transport in the near field of a repository on the basis of a network of 1dimensional drift structures. The focus of MARNIE lies on repositories in rock salt. It simulates advective-diffusive transport processes including hydrodynamic dispersion, the effect of gases on liquid transport, convergence of cavities with corresponding compaction of the backfill, container failure, radionuclide mobilisation and decay, solubility limits, sorption, and the impact of temperature.

FLAC3D

FLAC3D (Fast Lagrangian Analysis of Continua in 3 Dimensions) is a commercial explicit Finite Difference Code developed by Itasca Consulting Group. It can be used for all kinds of computational engineering mechanics, but it is focused on geotechnical problems. Elastic and plastic deformation for many types of materials (soils, rocks etc.) can be simulated with a variety of different constitutive relations. The basic version is capable to combine hydraulics and mechanics. For more complex situations add-on modules are available.

GRS currently uses the basic version combined with the Thermal, Creep and C++ add-on modules. This enables GRS to model thermal-hydro-mechanical processes for many different repository settings, e.g. for all probable host rocks (Soft Clay, Rock Salt, Hard Rock). Additionally, it is possible to extent the code either with self-developed C++ functions or by employing an easy to use intrinsic language in FLAC3D.

GRS has developed an extensive, carefully maintained, library of functions and add-on tools written in Perl, Python and C++ for FLAC3D. The possibility to easily extent, modify and develop codes has been used to couple FLAC3D with the multi–phase transport code TOUGH2. The C++ add-on allows GRS to use new published and reviewed constitutive relations as well as to develop our own or modify existing constitutive relations. Additionally, graphical pre- and post-processing capabilities of FLAC3D are used to visualize model output from TOUGH2.

<u>Spring</u>

SPRING is a commercial program system for the generation and calculation of groundwaterand mass transport models. It is based on the finite-elements-method. This system is used for complex problems and also for simple estimations by questions of flow, temperature and transport. The main areas for the application of Spring are geothermal aspects, waste disposal, groundwater resources management, permanent storage and mining.

Development of modelling capabilities

The future development will presumably involve the coupling of some above described





computer codes or new codes. For example the coupling of the TOUGH2 code with FLAC3D or geochemical codes with TOUGH2.

6.6 LITHUANIA

At the moment the main fields where LEI conduct R&D actions important for the safety case of DGR are:

- evaluation of the source term (SNF, ILW), its radiological and thermal characteristics (inventory),
- modeling of SNF criticality,
- modeling of dose rate at the canister surface and at some distance,
- assessment of dose to the personnel and population during the operational phase of disposal facility,
- modeling of heat transfer from the waste container in disposal facility,
- modeling of radionuclide transport through the engineered and natural barriers (transport in liquid and gas phase),
- modeling of radionuclide transport and distribution in the biosphere,
- assessment of radiological consequences for the humans,
- development and analysis of scenario, conceptual models,
- assessment of the uncertainties and sensitivity analysis.

Evaluation of the source term for SNF or any other type of radwaste disposal is probably the most critical thing to consider. Heat generation and overall radiation characteristics of the SNF are usually the ones that determine design of the SNF disposal canisters and their layout in the repository, whereas the list of radionuclides presented in the SNF and their activities are very important for modelling of possible radionuclides transport from the repository. LEI's experts have experience and capabilities for numerical evaluation of the source term in all these aspects:

- decay heat generation of SNF can be modelled for any time period, providing total, gamma, beta heat generation, etc.;
- gamma and neutron fluxes can be evaluated for any time period, providing total fluxes as well as grouped into desired energy ranges;
- list of light elements, actinides and fission products can be obtained providing specific and total activities of each radionuclide for any time period.

The source term in these aspects can be evaluated not only for SNF itself, but also taking into account radionuclides presented in the structural parts of SNF assemblies (cladding, other assembly parts) and other type of waste, which are disposed off in the same repository as SNF.

All evaluations can be performed taking into account different properties of SNF fuel being disposed of (different initial enrichment, burnable absorber content, burnup depth, irradiation and cooling time, etc.). Criticality safety evaluations can be performed with or without implementation of the burnup credit. The capabilities to evaluate the inventory of





SNF with high burnup and its criticality need to be developed/improved.

State of the art computer codes that are widely used across the world are in the disposition of LEI's experts – MCNP/MCNPX codes and SCALE codes system. In order to improve the efficiency and accuracy of modeling results the optimization of modeling process with those codes need to be improved.

As it has already been mentioned heat generation and distribution through the repository structural components and surrounding host rock are the characteristics that need to be considered during the development and justification of the design of SNF disposal canisters and repository layout. LEI experts has an experience and capabilities to evaluate decay heat transfer and distribution around the repository considering the source term and its evolution with time, rock specific properties (thermal conductivity, specific heat, material density, etc.), saturation, the actual geometry of repository components and surrounding geological media.

For the evaluation of thermal characteristics (e.g. modelling of temperature evolution) in deep geological repositories a computer code ANSYS/FLUENT could be applied, which is available in LEI and being used by LEI experts. ANSYS/FLUENT is the world leading CFD code for a wide range of modelling fluid flow and heat transfer in simple and complex 2D or 3D geometries. Heat transport by convection, conduction and radiation can be modelled by this software considering the specific material properties, source term, initial and boundary conditions.

In relation to the repository construction the present conditions in term of mechanical strains, groundwater movement regime, and temperature distribution will be affected. Various processes occurring in the engineered and natural materials may me strongly coupled and non-linear. Recently, the demand for the performance assessment of geological nuclear waste repositories has driven the development of coupled thermo-hydromechanical (THM) numerical models in the fields of rock and soil mechanics. LEI experts have some experience in modelling coupled THM processes, evaluation of gas flow through the engineered and natural barriers, its impact on barrier behaviour. The competence in modeling the complex system behaviour needs to be further developed constantly accompanied with knowledge being gained during the experimental work. Improved knowledge will allow more realistic analysis of the repository design and optimisation, and assessment of possibilities of radionuclide release and transport in the dissolved/gaseous phase.

Evaluation of possible humans' external exposure from the radiation coming from the SNF disposal casks and disposal facility itself is also very important during operational phase of the disposal facility lifetime. For workers, the direct radiation coming from the radiation sources is mostly important, whereas exposure evaluation of the population usually should additional account and radiation which is reflected from the sky/air (so called SKYSHINE effect). The ALARA principle should also be implemented in the overall repository operation design.

LEI's experts have experience and capabilities for numerical evaluation of the radiological consequences for the humans from the external radiation, accounting exposure coming from the neutrons and gammas, direct and reflected. The MCNP/MCNPX, Visiplan,





MicroShield, MicroSkyshine codes and SCALE codes system are available for these evaluations.

As a part of safety assessment or safety review the analysis of radionuclide transport from the repository is performed usually. This is a complex task which requires a comprehensive analysis of the repository performance as a whole, safety functions being fulfilled by separate components, their evolution in time, consideration of various features, events, processes leading to certain repository evolutions (scenarios). For scenario development one the common approaches (a top-down approach based on FEP's analysis) is used by the experts of LEI Nuclear Engineering Laboratory. Current experience and capabilities should be increased by increasing the competence of development of updated FEP databases, scenario development by analysing the state of safety functions.

For the developed conceptual models of radionuclide transport through the engineered and natural barriers a different approaches are applied considering the specific aspect of particular case. LEI experts have the capabilities to model groundwater flow, reactive radionuclide transport by diffusion and/or advection by applying the porous medium approach, discrete channel network approach. The main software available in LEI for this type of analysis is computer codes AMBER, DUST, GENII, GWSCREEN, GoldSim, Petrasim, Comsol, Compulink, CHAN3D, PREBAT-BATEMAN. Analysing the contaminants distribution /accumulation within the components of biosphere (surface water, soil, plants, animals) various physical, chemical processes are considered. The assessment of radiological consequences of radionuclide release from the repository is performed following the identified potential exposure pathways (inhalation, ingestion of contaminated food, water, soil particles, external exposure, etc.). In order to increase the confidence in performing or reviewing safety assessment/safety case, the competence of experts on the evaluation of representative geological data, interpretation of temporal and spatial variable data, results of short-term experiments need to be improved. The common approach for the managing of uncertainty related to long-term changes in nature is necessary for experts reviewing safety case. The deep knowledge and understanding are needed in case of radionuclide release mechanisms and rates from various radioactive waste (intermediate level waste, SNF), because there is a lack of experimental works on RBMK type SNF and ILW.

The confidence in the modeling results is built by performing uncertainty analysis by performing modeling in probabilistic manner included into the performance codes GoldSim, AMBER. In case of geological repository the sources of uncertainty are related to the uncertainty of scenario, models and parameters. Considering different type (irreducible, reducible) these uncertainty need to be managed and treated in safety assessments.

For the identification of the key aspects related to the repository safety the sensitivity analysis is performed by researches by application of different sensitivity analysis methods (differential, scatterplot, regression, correlation, etc.) with the means of general (Matlab) or specific software (GoldSim, SIMLAB). While evaluating of the priorities in further R&D at different stages of the repository based on the sensitivity and uncertainty analysis, an approach acceptable internationally is required by experts on the assessment end-points at each stage of repository programme, acceptable level of confidence, treatment of the uncertainties in the biosphere which are strongly related to the climate change during post-





closure period. In case of probabilistic assessment there is a need of common recommendation on the definition of probability distribution function for the parameter which is poorly measured. The results of sensitivity analysis form a basis for the priorities for subsequent research and development and play an important role in the uncertainty management. The competence of LEI experts needs to be improved in the application of other methods (like variance-based methods, etc.) in order to gain reliable knowledge and understanding of complex system behaviour and to perform sensitivity analysis in a systematic way.

For the evaluation of cost to plan, build and operate, close the repository, to conduct related research and development, a systematic assessment is needed. Based on Swedish methodology the generic assessment of cost of geological repository was carried out while analysing the possibilities to dispose SNF in crystalline rocks in Lithuania. The method used according this methodology is based on the application of the calculation principle called "successive principal". The central aspect of "successive principle" is the methodology for structuring the calculation and setting up its probability distributions. The total cost is obtained by adding items according to the rules that apply to addition of stochastic variables. The given results are then presented as a distribution function indicating the probability associated with a given cost. The method also provides indications of where the major uncertainties are. Some experience gained during this study allowed getting some knowledge about this type of assessment, but the competence needs to be improved considering other methodologies, managing the various activities related to the repository development and implementation.

6.7 NETHERLANDS

The Dutch concept for a Deep Geological Repository (DGR) for disposal of radioactive waste is still being developed. In the Netherlands attention mainly has been focused on suitable salt domes in the northern part of the country and Boom clay layers in the south and central part. The realization of a suitable concept is presently not a critical issue since the Dutch radioactive waste will be stored in a dedicated surface facility for a period of at least 100 years. However there have been several options investigated in the Netherlands, mainly within the former PROSA and CORA programmes (focus mainly on rock salt), and the currently running OPERA program (Boom clay). The different options include the concept of retrievability.

6.7.1 Previous modelling efforts

In the past several modelling efforts were performed in the framework of a variety of programmes and projects. Examples of these efforts for a salt-based repository are:

 Release and transport of radionuclides, including uncertainty/sensitivity analyses, using EMOS (EU-FP5 project BENIPA). EMOS (Endlagerbezogene MOdellierung von Szenarien) has been developed by GSF (Forschungszentrum für Umwelt und Gesundheit GmbH), Germany, for the assessment of radionuclide dissolution in a nuclear waste repository in rock salt, the subsequent nuclide transport from the





waste containers through the repository into the geosphere, and the distribution of the radionuclides in the biosphere.

- Assessment of the three-dimensional temperature distribution in salt host rock as a result of the heat input from HLW containers, using TASTE (EU-FP5 project ESDRED). TASTE (Three-dimensional Analysis of Salt dome Temperatures) has been developed by ECN/NRG, Netherlands, and is based on an analytical model of a continuous timedependent point source in an infinite solid of homogeneous isotropic material with temperature independent properties.
- Assessment of compaction processes of salt grit backfill, and compacted salt sealing plugs, using EMOS (EU-FP5 project BAMBUS-II; EU-FP6 project PAMINA). NRG developed models to characterize this compaction behaviour and implemented these models into EMOS. The models are based on experimental results from compaction tests performed at the Utrecht University. Within PAMINA uncertainty/sensitivity analyses were performed applying these models.
- Safety assessment of the Asse mine, using LOPOS, in cooperation with GRS Braunschweig (Germany) and Colenco (Switzerland). LOPOS has been developed by GRS, Braunschweig, and models the release of radionuclides from waste packages, their transport through repository flow paths, and the subsequent uptake in the biosphere.

Examples of previous modelling efforts for a clay-based repository are:

- Simulations of the release and transport of radionuclides through bentonite barriers and Boom Clay, using PORFLOW (EU-FP5 project BENIPA). PORFLOW, which has been developed by Analytic and Computational Research Inc. (ACRi), is a comprehensive mathematical model for the steady-state or transient simulation of multi-phase fluid flow, heat transfer, and mass transport processes in variably saturated porous and fractured media
- Assessment of the release and transport of radionuclides through Boom Clay, including uncertainty/sensitivity analyses, using PORFLOW (EU-FP6 project PAMINA).
- Performance of THM post-test analyses on the small scale in-situ heater experiment ATLAS (Admissible Thermal Loading for Argillaceous Storage), and pre-test analyses on the large-scale heater test PRACLAY, both performed in the underground laboratory HADES in Mol. The analyses were done with FLAC-3D in the framework of the EU-FP6 project TIMODAZ. FLAC-3D (Fast Lagrangian Analysis of Continua in 3 Dimensions) is a commercial explicit Finite Difference Code developed by Itasca Consulting Group.

6.7.2 Present modelling efforts

The present section summarizes the most important modelling efforts performed within the OPERA program. As stated previously, the research executed in OPERA concentrates on a deep geological disposal facility in Boom Clay host rock.





6.7.2.1 WASTE CHARACTERIZATION

Changes in the presently adopted nuclear fuel cycle strategy in the Netherlands may impact both the quantities of generated radioactive waste as its composition: for the production of nuclear energy, several technological and logistic options are possible, i.e. reprocessing of waste, the utilisation of MOX-fuels in current reactors, the deployment of gas-cooled high temperature reactors (HTRs) or other 3rd or 4th generation technologies, including fast breeder reactors. The computer code DANESS (*Dynamic Analysis of Nuclear Energy System Strategies*) has been adopted to quantify the consequences for several possible alternative nuclear fuel cycle scenarios in terms of waste amounts and compositions. DANESS, which has been developed by Listo B.V (Belgium), is an integrated dynamic nuclear process model for the analysis of today's and future nuclear energy systems and for the simulation of the flows of fissile material, fresh fuel, spent fuel, high level waste, all intermediate stocks, and amounts and isotopic composition of radioactive waste in the final disposal facility.

6.7.2.2 THM PHENOMENA

Within the OPERA research program, a consortium formed by the Delft University of Technology, the Netherlands Organisation for Applied Scientific Research (TNO), and NRG, will analyse the performance of the Dutch repository concept in Boom Clay by computing the deformations and stability during staged excavation and construction of the underground facility. The influence of transient hydraulic and thermal effects in the pre- and post-closure assessments will be analysed using the geotechnical finite element code PLAXIS 3D. Several constitutive models for soil behaviour will be tested and developed further, including anisotropic creep models. The aim of the research is to develop a dedicated model for Boom clay.

In addition, so-called "approximate" probabilistic tools, such as the First Order Reliability Method (FORM), will be used to conduct reliability-based sensitivity studies accounting for parameter uncertainty. This tool will be integrated into the PLAXIS code, making PLAXIS applicable to conduct finite element sensitivity studies within a probabilistic framework. This integration allows an assessment of the repository performance uncertainty; and an objective means by which the relative importance of parameters may be assessed.

6.7.2.3 GEOCHEMICAL BEHAVIOUR OF THE ENGINEERED BARRIER SYSTEM

The objective of this project, performed by NRG, Deltares, and TNO, is to provide an overview of the state-of-the-art scientific knowledge on relevant geochemical, microbial corrosion and degradation processes in the engineered barrier system (EBS) and waste matrix of the Dutch generic repository design in Boom Clay. Examples of such processes are the corrosion behaviour of vitrified waste, corrosion behaviour of spent fuel, non-thermal HLW, and LLW/ILW, metal corrosion processes, cementitious material degradation, and microbiological effects on the EBS and Boom Clay.

The main focus of this project is to elaborate whether certain (geo-)chemical interactions influence the assumptions and modelling approaches of the long-term safety assessment of the disposal facility.





6.7.2.4 GEOLOGICAL MODELLING

The modelling of the hydrostratigraphy of the overburden of the Boom Clay, i.e. the overlying hydrostratigraphical units (aquitards and aquifers), will be mainly based on the existing nation-wide hydrogeological model REGIS II.1⁷, as developed at TNO (Netherlands Organisation for Applied Scientific Research). The conceptual model will include information on the tectonic history by means of fault offsets (possibly of influence as flow barrier). Additional assessments on relevant geodynamic history, such as determination on maximum burial and erosional thicknesses (required for property analysis) is addressed with burial history modelling tools.

6.7.2.5 GEOHYDROLOGICAL CHARACTERIZATION OF THE BOOM CLAY

Existing lab and in situ porosity and permeability measurements of the Boom Clay will be combined with the updated lithological and lithofacial concepts to derive a regional scale conceptual model of present porosity lateral and vertical permeability distributions within the Boom Clay, including an estimation of the uncertainty range. The geohydrological characterization of the overburden will be mainly based on the above-mentioned REGIS II.1 model.

6.7.2.6 GEOCHEMICAL INTERACTIONS IN BOOM CLAY

In a joint effort, TNO and NRG will study the geochemical short- and long-term evolution of Boom Clay as affected by heat, gas generation and corrosion/degradation products of the engineered barrier system. For the evaluation of these potential interactions the thermo-hydraulic modeling codes TOUGH2 and the version coupled with geochemistry TOUGHREACT will be applied. In addition the computer code ORCHESTRA⁸ will be ulitized, which can handle very detailed geochemical interactions, including speciation, redox chemistry, the presence of charged surfaces, chemisorption and precipitation. This allows to study in detail trace element interactions with clay, oxide and organic rock/soil particles.

6.7.2.7 RADIONUCLIDE MIGRATION

For the long-term safety of the OPERA reference concept for radioactive waste in Boom Clay, the migration behaviour of radionuclides in the host rock is the most relevant safety function. The physical-chemical mobility of radionuclides in Boom Clay will be analysed by assessing the role of underlying fundamental processes that are relevant in relation to the partition of radionuclides over the mobile and immobile (solid) phases and the transport of radionuclides in or with the mobile phase. The sorption and precipitation behaviour of radionuclides will be evaluated, the role of diffusion in the complex, heterogeneous Boom Clay will be analysed, and the potential role of colloids for migration will be addressed.

These efforts will be facilitated by making use of the ORCHESTRA modelling framework.

SITEX

⁷ http://www.tno.nl/downloads/uGB%20085-11-09.pdf

⁸ ORHESTRA: Objects Representing CHEmical Speciation and TRAnsport models, http://www.meeussen.nl/orchestra/





6.7.2.8 RADIONUCLIDE MIGRATION IN THE SURROUNDING ROCK FORMATIONS

In the event radionuclides reach the boundaries of the host formation and enter the overburden or those aquifers under the Boom Clay that are connected to the overburden at the national scale, the safety function "dilution and dispersion" comes into play. In order to assess the contribution of this safety function to the overall safety of the concept of geological disposal of radioactive waste, the extent to which concentrations are reduced by radioactive decay, dilution and dispersion has to be quantified.

As part of the OPERA program the Dutch National Hydrological Model Instrument (NHI⁹), the state-of-the-art groundwater flow model of the Netherlands, will be extended with a hydrological modelling approach that considers the geohydrological situation of the Netherlands on the national scale and which establishes simplifications on the hydrological controls on groundwater transport. In addition, research will be carried out on the biogeochemical processes that control the reactive behaviour of the radionuclides, focusing on the most mobile radionuclides. The final result is a modelling approach for transport of mobile radionuclides that contains a simplification on the controlling physico-chemical processes and is representative for the hydrogeological settings of the Netherlands.

6.7.2.9 SAFETY ASSESSMENT

The long-term safety assessment of the Dutch generic disposal facility design in Boom Clay will be performed in a consortium led by NRG with the ORCHESTRA modelling framework. ORCHESTRA is being applied since (1) the code is capable to represent correctly all current state-of-the-art sorption models; (2) its open, object-oriented structure which can be expanded to cover potential model improvements and/or modifications that will be developed during the OPERA program ; (3) the code allows to link complex process-oriented fundamental models with its simplified PA model representation in an efficient way; (4) unlike other modelling codes, it enables to exactly represent the modelling algorithms developed in other OPERA projects rather than only approximate them.

ORCHESTRA will comprise a calculational framework for the transport of radionuclides from a deep geological repository for the final disposal of radioactive waste through the rock formation surrounding the near field of the repository and to the biosphere, as well as the subsequent uptake by the living environment.

The safety assessment will include a probabilistic uncertainty/sensitivity analysis of a variety of evolution scenarios of the repository.

6.7.2.10 FURTHER DEVELOPMENT

The presently running OPERA program addresses all major aspects that nowadays are considered to be relevant for the long term safety of a deep geological disposal facility implemented in a Boom Clay host rock environment in the Netherlands. Upon the finalization of the OPERA program in 2015 an evaluation will be performed of the accomplished research efforts which may lead to recommendations for further work to guarantee the long term safety of deep geological disposal.

SITEX

⁹ http://www.nhi.nu/nhi_uk.html





6.8 SLOVAKIA

6.8.1 DECOM, a.s.

The main software codes available at DECOM, a.s. related to R&D of Deep Geological Disposal of radioactive waste are GoldSim and Amber.

GoldSim code (together with RT an expanded version of the Contaminant Transport Module) is integrated modelling tool, which is used as a standard code for conduction of safety analyses. Another integrated models are developed in AMBER code.

Except of DECOM, a.s. a number of organizations has been involved in DGR safety case development and safety calculations in Slovakia e.g. VUJE, a.s., State Geological Institute of Dionýz Štúr. Besides, foreign companies (e.g. UJV Řež, a.s.) provided services and performed safety studies particularly in the area of source term and near-field modelling.

Any of these organisations could provide support to Nuclear Regulatory Authority in its decision making process and reassess the safety cases for reviewing purposes.

6.8.2 VUJE, a.s.

The R&D activities of VUJE are related primarily to near surface repository and radiation safety of nuclear installations operation. However most of the skills are applicable also for DGR purpose. VUJE, a.s. owns and has long-term skills in utilization of following codes:

- GoldSim
- Hydrus
- Modflow
- ORIGEN, SCALE, HELIOS.

6.9 SUMMARY

The summary of modelling capacities, available for each beneficiary to cover specific R&D issues is listed in Tab. 5.



Community research Tab. 5. The summary of modelling capacities, available for each beneficiary to cover specific R&D issues

	Beneficiar Y	RadProtection/ Inventory	Heat transfer	Geochemistry	Geomechanics	Transport, migration	Safety assessment	Future actions
	BELV FANC	RadProtection: MCNPX		PHREEQC		HYDRUS 1D, HYDRUS 2D STANDARD	MELODIE (IRSN), batch calc., sensitivity analyses (own code)	
	CNSC		COMSOL		COMSOL	MODFLOW, CORMIX		
	UJV Rez	Inventory: SCALE, ORIGEN 2.2	TOUGH2	PHREEQC, GWB, TOUGHREACT		TOUGH2, FEFLOW	PAGODA, Amber,	Influence of simplification of system in SA models
_	IRSN	RadProtection: SYMBIOSE, AQUAREJ, FOCON 96, ISIS (fire)		PHREEQC, HYTEC	CASTEM, LAGAMIN	DIPHOM, nSIGHTS (hydraulic tests)	MELODIE	
	GRS		TOUGH2	PHREEQC	FLAC3D	TOUGH2, MARNIE, FLAC3D, Spring		Coupling of TOUGH2 with FLAC3D or with gch code







Beneficiar Y	RadProtection/ Inventory	Heat transfer	Geochemistry	Geomechanics	Transport, migration	Safety assessment	Future actions
LEI	Inventory: MCNPX, SCALE RadProtection: MCNPX, Visiplan, Microshield, MicroSkyshine, SCALE	ANSYS/ FLUENT		COMSOL	AMBER, DUST, GENII, GWSCREEN, GoldSim, Petrasim (TOUHG2), COMSOL, COMSOL, Compulink, CHAN3D	AMBER, DUST, GENII, GWSCREEN, GOLDSIM, COMPULINK, CHAN3D	THMC processes
NRG	Inventory: DANESS RadProtection: MCNPX, Visiplan, Microshield, MicroSkyshine, SCALE	TASTE	TOUGHA2, TOUGHREACT ORCHESTRA	EMOS (compaction)	EMOS, REGIS II.1, ORCHESTRA	EMOS, LOPOS, PORFLOW, ORCHESTRA	тнмс
DECOM	ORIGEN, Scalem Helios (cooperation)				MODFLOW, HYDRUS (VUJE)	GOLDSIM, AMBER	

^* * *^

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7 Determination of capabitility to cover R&D needs for knowledge, identified in the D3.1

In deliverable D3.1 [1] the following list of general R&D needs for knowledge, reflecting the common view of participants on the key actions that should guide the development of a more detailed R&D programme for a future TSO network, was identified.

- A1 To assess the accuracy and the exactitude of methods available for the evaluation of data necessary for long-term and operational safety demonstrations.
- A2 To assess if the data evaluated at small scale (in time and space) are representative of the in situ repository conditions and future evolution.
- **B1** To develop independent understanding in the processes on which rest the performances of the waste form.
- **B2** To develop independent understanding in the processes on which rest the performances of the waste canister and its overpack.
- **B3** To develop independent understanding in the processes on which rest the performances of the Engineered Barrier System (EBS).
- **B4** To develop independent understanding in the processes on which rest the performances of the Geosphere.
- **B5** To develop independent understanding in the internal perturbations of the disposal system resulting from the waste/host-rock and waste/EBS interactions.
- **B6** To develop independent understanding in the internal perturbations of the disposal
- **B7** To develop independent understanding in the internal perturbations of the disposal system resulting from potential operational transients.
- **B8** To develop independent understanding in the potential external perturbations of the disposal system.
- **C1** To evaluate the reliability of methodologies followed by the operators for the assessment calculations.
- **C2** To develop independent models in order to evaluate the extent, the intensity and the radiological impact of processes resulting from internal and external perturbations of the repository
- **C3** To evaluate the methodology followed by operators for managing the uncertainties surrounding the safety assessments.
- **C4** A methodology to review the hazards possibly occurring in an underground nuclear facility and scientific basis associated to development of conventional/nuclear hazardous processes underground
- **C5** Definition of the reference state of the system (normal/expected evolution) and monitoring methods in order to detect deviations







The additional goal of D3.2 is to identify which topics are covered by enlisted research laboratories and installations and by modelling tools, available for participants for potential future R&D needs for knowledge.

7.1 QUALITY OF INPUT DATA

7.1.1 Methodology adequacy and relevance

Identified R&D needs for knowledge:

A1 To assess the adequacy and relevancy of methods available for the evaluation of data necessary for long-term and operational safety demonstrations.

- Method to characterize the source term
 - Currently available: IRSN (bitumen inventory); SF: UJV, DECOM (VUJE)
 - o Will be performed: IRSN bitumen
 - Needed: vitrified waste source term
- Method to characterize DGR thermal development
 - Currently available: experiments: UJV Rez (in-situ experiment)
 - Can be performed:
 - Needed:
- Method to characterize container corrosion rates
 - o Currently available: experiments: UJV Rez (lab)
 - Will be performed: IRSN (lab, in-situ)
 - Needed: in situ experiments in granite
- Method to characterize the geo-mechanical properties of the host-rock (advanced coupled (T)HM behaviour)
 - o Currently available: CNSC
 - Will be performed:
 - Needed: more development is needed; competence development
- Method to characterize diffusion properties of the near-field materials and the host-rock
 - Currently available: UJV Rez (buffer lab, host rock lab, in-situ), CNSC (cooperation); IRSN (lab, in-situ)
 - Will be performed:
 - Needed: competence development
- Method to identify transport properties of the host rock (faults and joints)
 - Currently available: IRSN (lab, in-situ), UJV (basic level)
 - Will be performed:





- Needed: more development is needed for crystalline rock; competence development
- Method for description of geological properties of the site
 - Currently available: IRSN; generally it is performed on the basis of subcontracting, knowledge is available; CNSC has geoscience advisory panel
 - Will be performed:
 - Needed: competence improvement to deal with properties variability
- Method to evaluate the sorption capacity of the near-field materials and the host-rock
 - Currently available: UJV (lab near field, rock; in-situ rock); IRSN (lab, insitu - Mt. Terri)
 - Will be performed:
 - Needed: modelling competence development, model validation based on experimental data
- Method to evaluate the permeability of near-field materials and the host-rock
 - Currently available: UJV (lab, in-situ), IRSN (lab, in-situ)
 - Will be performed:
 - Needed: competence improvement

7.1.2 Representativeness of the evaluated data

DGR is a large complex multibarrier system, being constructed in heterogeneous host rock massives. Therefore not all the information can be easily generalized. Data can suffer from both simplification of complex system, processes and time scales and from size reduction, namely due to laboratory research. Therefore the data may not be fully representative of the whole DGR system and its future evolution. Consequently, TSOs and safety authorities should develop confidence in:

- the upscaling approaches for the data evaluated at small scale in order they can be representative for the whole DGR system;
- methods for data extrapolation in time (e.g. for the long-term safety demonstration);
- methods, dealing with system heterogeneity.

Confidence in the transferability and in the time extrapolation in terms of data for the safety demonstration may notably be build by understanding the complex processes and phenomena that will alter the evaluated data under repository conditions (see section 6.2). The coupling between the Thermal, Hydrological, Mechanical and Chemical (THMC) properties of the DGR system is of particular concern for the transferability and the extrapolation in time of the evaluated data.

Identified R&D needs for knowledge:

A2 To assess if the data evaluated at small scale (in time and space) are representative for in situ repository conditions and future evolution.





- Representativeness of rock properties (mineralogy and petrology, porosity, pore connectivity, fracturing, mechanical properties, thermal properties)
 - Currently available: UJV (lab porosity, heat, mineral heterogeneity), CNSC (lab mechanical properties)
 - Will be performed: CNSC (hydraulic conductivity)
 - Needed: more development is needed; competence development
- Representativeness of hydraulic performance of seals and concrete liners
 - o Currently available:
 - Will be performed: IRSN+CNSC
 - Needed: question if it is needed, competence development on material degradation
- Representativeness of the geological structures in 3D dimensions (e.g. seismic methods)
 - Currently available: IRSN (can be shared)
 - Will be performed:
 - Needed:
- Representativeness of barriers transport properties (sorption, diffusion data, permeability)
 - Currently available: UJV (lab, in-situ crystalline), IRSN (lab, in-situ clay rock)
 - Will be performed
 - Needed: competence improvement on upscaling, dealing with variability

7.2 UNDERSTANDING OF COMPLEX PROCESSES

In order to design the GD facility and to demonstrate its long-term and operational safety, operators have to develop understanding of the key processes (i.e. Thermal, Hydrological, Mechanical and Chemical processes and their related couplings) which govern the evolution of the GD system. TSOs and safety authorities have to build confidence in the understanding developed by the operator. This may be achieved notably by undertaking independent R&D needs for knowledge devoted to the understanding of:

- the processes on which rest the performances of the four main components of the disposal system (waste forms, canister and overpacks, Engineered Barrier System (EBS) and geosphere);
- the processes resulting from potential internal and external perturbations of the disposal system (i.e. its long term stability).

For these two topics, R&D needs for knowledge are described in the two following subsections. The understanding of the (individual and coupled) processes might require complex experiments, large computing resources and time. Consequently, the priority might be in the development of small scale experiments and models. Need for knowledge A2 (see

SITEX





section 6.1.2) should give confidence in the upscaling of the acquired data and models to conditions representative of the disposal system.

7.2.1 Processes on which rest performances of individual components

This subsection defines R&D needs for knowledge aiming at characterizing the processes on which rest the performances of the four main components of the disposal system (waste forms, canister and overpacks, Engineered Barrier System (EBS) and geosphere).

7.2.1.1 WASTE FORMS

Identified R&D needs for knowledge:

B1 To develop independent understanding in the processes on which rest the performances of the waste form.

Particular points of attention (not exhaustive list):

- SNF disposal: characterization of the process responsible for the Instant Released Fraction (IRF) notably due to ¹²⁹I and ³⁶CI
 - Currently available: calculation UJV Rez (to be confirmed)
 - Will be performed:
 - Needed: measurement technique should be involved and developed, knowledge of processes, competence on method evaluation, results interpretation
- Graphite bearing wastes (e.g. RBMK, UNGG reactor type): characterization of processes responsible for the ¹⁴C and ³⁶Cl release from waste forms
 - Currently available: LEI modelling of C-14 transport from RBMK-1500 graphite
 - Will be performed: LEI modelling of C-14 release and transport from RBMK-1500 graphite considering Lithuanian specific conditions
 - Needed: mechanistic model of C-14 release based on graphite leaching data
- Vitrified waste: influence of the initial fracturing state of glass on its dissolution rate (and thus the radionuclide release rate)
 - o Currently available: IRSN; UJV (analogue desk study)
 - Will be performed:
 - o Needed:
- The dissolution rate of the vitrified waste packages (e.g. influence high pH from the concrete environment)
 - o Currently available: IRSN; UJV (analogue desk study)
 - Will be performed:
 - Needed:
- Influence of dissolutions rates for radionuclide release from SNF (influence pH, Eh,

SITEX





oxidation/redox conditions)

- Currently available: UJV (lab studies; natural analogue study)
- Will be performed:
- Needed: competence improvement on radionuclide dissolution modelling
- Bituminised waste
 - Currently available: UJV (half scale bituminisation facility, leaching studies)
 - Will be performed:
 - Needed: need to be developed (IRSN, BEL V)

7.2.1.2 CANISTER & OVERPACK

Identified R&D need for knowledge:

B2 To develop independent understanding in the processes on which rest the performances of the waste canister and its overpack.

- The influence of the thermal dissipated power on the canister and overpack properties
 - o Currently available: UJV Rez (partly)
 - Will be performed:
 - Needed: needs to be developed for material needed, competence development
- The assessment of corrosion mechanisms and rates (e.g. generalised or pitting corrosion) in reference conditions
 - Currently available: UJV Rez, IRSN
 - Will be performed:
 - Needed: competence development
- The dimensioning of the canister and overpack with respect to the different loads experienced under repository conditions (due to the host-rock behaviour and to the thermo-mechanical effects)
 - Currently available: construction company
 - Will be performed:
 - Needed: needs to be developed, basic knowledge to evaluate conditions and premises during dimensioning
- The influence of corrosion layer on the extent of corrosion
 - o Currently available: UJV Rez
 - Will be performed:
 - Needed: knowledge on corrosion processes during pre-disposal stage and their extend
- Influence of microbiota on corrosion rates
 - o Currently available: IRSN (lab, in-situ)





- Will be performed:
- Needed: need to be developed

7.2.1.3 ENGINEERING BARRIERS (BUFFERS AND SEALS, CONSTRUCTION MATERIALS)

Identified R&D need for knowledge:

B3 To develop independent understanding in the processes on which rest the performances of the Engineered Barrier System (EBS).

Particular points of attention (not exhaustive list):

- Processes affecting the geo-mechanical properties of the EBS (swelling capacity of bentonite materials, change of the chemical composition of bentonite materials...)
 - Currently available:
 - o Will be performed: CNSC
 - Needed: competence development on geomechanical modelling
- Process affecting the hydraulic properties of the EBS (EBS permeability...)
 - o Currently available: UJV Rez, IRSN
 - o Will be performed: IRSN
 - Needed: competence development
- Processes of buffer erosion (causing lost of the performance)
 - o Currently available: UJV Rez (basis, colloid), IRSN
 - Will be performed:
 - o Needed: competence development
- Processes on which rest the retention/sorption capacity of the EBS
 - o Currently available: UJV Rez (lab), IRSN (concrete)
 - Will be performed:
 - Needed: competence development
- Interaction processes at the material border of materials (buffer/container; buffer/host rock)
 - Currently available: UJV Rez, IRSN
 - o Will be performed: UJV Rez
 - Needed: **need to be developed;** competence development
- Long term evolution of buffer and sealing materials (long term tests, natural analogues)
 - o Currently available: IRSN
 - o Will be performed: IRSN
 - Needed: need to be developed; competence development on durability evaluation

7.2.1.4 GEOSPHERE





Identified R&D need for knowledge:

B4 To develop independent understanding in the processes on which rest the performances of the Geosphere.

- Long term stability of the geosphere (including seismic, orogenic properties)
 - o Currently available: IRSN
 - Will be performed:
 - Needed: the field of geology: needs to be developed??
- Processes affecting the mechanical properties of the geosphere and its healing (for clay rock and rock salt)
 - Currently available:
 - Will be performed: IRSN
 - o Needed: competence development
- Influence of the mineralogical composition of the host rock on its sorption capacity.
 - o Currently available: UJV Rez partly (lab, in-situ)
 - Will be performed:
 - Needed: competence development
- The migration of radionuclides in the host-rock at ambient temperature and considering temperature gradient representative of those that may occur in the near-field of the foreseen waste disposal system
 - Currently available: IRSN (lab, in-situ); UJV Rez (without influence of T; lab, in-situ)
 - Will be performed:
 - Needed: increased competence in radionuclide transport by modelling migration experiments
- Identification of fracture wetting surface in fractured rocks in order to determine the extent of radionuclide migration
 - o Currently available:
 - Will be performed: UJV (maybe in future)
 - Needed: **need to be developed;** competence development
- Evaluation of indicators on the confinement capacity (i.e. diffusion dominated) at long-term, and its consistency with the DGR concept
 - Clay type DGR: verification that the concentration of solutes (such as Cl) shows a classical diffusion profile, which proves that diffusion prevailed up to present day (i.e. before DGR implementation); identification of effective porosity, i.e. the porosity available for radionuclide migration
 - Currently available: IRSN, CNSC
 - Will be performed:
 - Needed: competence development/improvement on measurement methods and result interpretation
 - Granitic type DGR: identification of pore connectivity in the crystalline rock massives; identification of effective porosity, i.e. the porosity available for





radionuclide migration

- Currently available: UJV Rez (with other partners)
- Will be performed:
- Needed: need to be developed; competence development/improvement on measurement methods and result interpretation

7.2.2 Processes resulting from internal and external perturbations

- Internal perturbations:
 - Waste component/Host-rock and Waste/EBS interactions;
 - EBS/Host-rock interactions;
 - Perturbations during the operational phase;
 - Perturbations due to constructions
- External perturbations.

7.2.2.1 INTERNAL PERTURBATIONS: WASTE COMPONENTS/HOST-ROCK AND WASTE/EBS INTERACTIONS

Identified R&D need for knowledge:

B5 To develop independent understanding in the internal perturbations of the disposal system resulting from the waste/host-rock and waste/EBS interactions.

Particular points of attention (not exhaustive list):

- Effects from waste forms:

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- The compatibility between bitumen waste and the surrounding concrete and host-rock (with respect to their potential swelling)
 - Currently available: UJV Rez (partly)
 - Will be performed:
 - Needed: need to be developed (IRSN, BEL V)
- Generation of gases (H₂, O₂) upon radiolysis of pore water, microbiological degradation of organic-based waste (e.g. bitumen)
 - Currently available: IRSN/BEL V
 - Will be performed:
 - Needed: need to be developed
- Radiation effects on materials
 - Currently available: IRSN
 - Will be performed: UJV Rez
 - Needed: competence improvement to evaluate proper selection of materials
- The gas issue

- Gas release from waste packages and from the corrosion or radiolysis of engineered barriers
 - Currently available: UJV Rez, IRSN
 - Will be performed:
 - Needed: increased knowledge on gas release modelling

SITEX





- The study of the generation and migration of gas from the waste repository
 - Currently available: CNSC, LEI (some experience on modelling of TH, THM)
 - Will be performed:
 - Needed: competence improvement on gas transport modelling, model validations

7.2.2.2 INTERNAL PERTURBATIONS: EBS/HOST-ROCK INTERACTIONS

Identified R&D need for knowledge:

B6 To develop independent understanding in the internal perturbations of the disposal system resulting from the EBS/host-rock interactions.

- Effects due to the corrosion phenomenon:
 - The corrosion behaviour of steel-based material in an anaerobic environment of deep repository
 - Currently available: UJV Rez, IRSN
 - Will be performed:
 - Needed: competence development (LEI)
 - The clay materials evolution due to iron-clay interactions (characterisation and modelling)
 - Currently available: IRSN
 - Will be performed: UJV Rez, IRSN
 - Needed: competence development
 - Effect of interaction of bentonite/steel on corrosion layer development and influence on the corrosion rate
 - Currently available:
 - Will be performed: UJV Rez
 - Needed: competence development
 - Anaerobic corrosion of iron metals is in addition connected with gas generation that can be detrimental to other components of a repository
 - Currently available:
 - Will be performed:
 - Needed: need to be developed; competence development
- Effects due to alkaline perturbation:
 - The clay materials evolution due to cement-clay interactions by characterisation and modelling
 - Currently available: UJV Rez (in-situ), IRSN
 - Will be performed: IRSN
 - Needed: competence development on modelling
 - Mineral transformations of bentonite in the alkaline front environment (it relates mainly to composition of penetrating alkaline waters, pH, single minerals transformation trend)





- Currently available:
 - Will be performed: UJV Rez
- Needed: competence development (knowledge and modelling capability)

7.2.2.3 INTERNAL PERTURBATIONS DUE TO OPERATION AND CONSTRUCTION

Identified R&D need for knowledge:

B7 To develop independent understanding in the internal perturbations of the disposal system resulting from potential operational transients.

Particular points of attention (not exhaustive list):

- Effect of the oxidizing and desaturation transient process
 - Currently available: IRSN (in-situ), UJV Rez (analogue study)
 - Will be performed:
 - \circ Needed:
- Effects resulting from the presence of micro-organisms
 - Currently available:
 - Will be performed:
 - Needed: needs to be developed, competence development
- Influence of defects, caused by handling, on canister corrosion
 - Currently available:
 - Will be performed:
 - Needed: needs to be developed
- EDZ formation and extent
 - Currently available: UJV Rez (lab, in-situ), IRSN (lab, in-situ), CNSC (numerical modelling)
 - Will be performed:
 - Needed: **needs to be developed;** knowledge to support model development for radionuclide and gas transport

External perturbations

Identified R&D need for knowledge:

B8 To develop independent understanding in the potential external perturbations of the disposal system.

SITEX

- General geological condition change (potential marine transgression, future permafrost/glaciations, site erosion, site seismicity, site uplift/subsidence)
 - \circ $\,$ Currently available: CNSC (glaciation) $\,$
 - Will be performed:
 - Needed: needs to be developed or organized as complex project; competence to evaluate the main premises for further climate change scenario





- The changes of the properties of the natural and engineered barriers (through the changes in groundwater flow regime, chemical conditions) are strongly related to the condition changes which are expected in the future
 - o Currently available: UJV Rez (erosion of bentonite),
 - Will be performed:
 - Needed: needs to be developed; competence development (knowledge of phenomena extend, to be able to quantify changes reasonably)
 - Potential future human intrusion and activities (gas storage and extraction, geothermal energy, resources exploration etc.)
 - o Currently available: UJV Rez (calculation of intrusion scenario)
 - Will be performed:
 - Needed: need to be developed (IRSN); competence development on activities extend conceptualization

7.3 VERIFICATION OF EXTENT, INTENSITY AND IMPACT OF PROCESSES

7.3.1 Reliability of FEPs and scenarios

Identified R&D need for knowledge:

C1 To evaluate the reliability of methodologies followed by the operators for the assessment calculations.

- Features, events and processes that are potentially important for the safety of the disposal system should also be identified thus there is a priority suggested on the development of updated FEP databases. E.g.:
 - Scenario caused by earthquake leading to the immediate failure of various numbers of the canisters in the time of mean lifetime of canisters
 - Scenario caused by denudation or erosion leading to the substantial shortening of radionuclide pathways to the environment
 - Scenario caused by the formation of preferential pathways in part of buffer in boreholes with immediate failed canisters due to earthquake
 - Intrusion scenario leading to the failure of one canister and buffer immediately after the end of institutional control of the repository (300 years)
 - How to handle intrusion scenario with extremely low probability but high impact? Methodology is needed how to handle such a numbers in communication with the public.
 - Climate change scenario during post-closure period, taking into account evolution of the possible biosphere behaviour.
- Safety functions of all system components should be developed for scenario development
- FEP screening and scenario development should be supported by experimental demonstration and natural analogue observations





Currently available: expertise is broadly available through the participants (see Table with models)

Needed: broad discussion, more opinions would be desirable, comparison of approaches for scenario development with evaluations its prons and cons

7.3.2 Reliability of models

Identified R&D need for knowledge:

C2 To develop independent models in order to evaluate the extent, the intensity and impact of processes resulting from internal and external perturbations of the repository on human and the environment.

Particular points of attention (not exhaustive list):

- Relevance of underlying conceptual (phenomenological) models used for the performance assessment:
 - Source term model for the radionuclide release from waste packages and spent fuel. This modelling is of particular concern as it has a deep impact on the long term safety of radioactive waste disposal. As an illustration, the modelling of the spent fuel Instant Release Fraction (IRF) is an important point of attention (see "Data quality" section)
 - The modelling RN migration and sorption, account for the range of relevant geochemical processes
- Investigate the influence of the level of abstraction and simplification (of mechanical, hydrological, thermal and chemical processes) on the results of the assessment calculations; so as the robustness of the data transfer from one system component to the other
- Verification and validation of the models, both conceptual and mathematical ones

Currently available: expertise is broadly available through the participants (see Table with models)

Needed: THMC models and reactive transport modes (coupled) are desirable

7.3.3 Management of uncertainties

Identified R&D need for knowledge:

C3 To evaluate the methodology followed by operators for managing the uncertainties surrounding the safety assessments.

Particular points of attention (not exhaustive list):

- The uncertainties may be divided into the following categories:
 - Input data quality (see section 6.1)
 - The management of parameters (phenomenological models) uncertainty around a mean value
 - Uncertainty of abstraction/simplification of the reality leading to conceptual

70





models

- o Uncertainty of upscaling process and long-term extrapolation in time
- o Uncertainty of Mathematical representation of processes included
- Applied software and its verification and validation; confirmation of its suitability
- DATA: uncertainties evaluated by data producer; based on experimental procedure, uncertainty determination methodology and QA; who is produces the data, they have to handle the uncertainties, see need for knowledge A1 and A2; probabilistic and sensitivity modelling
- Models: to use different model and verify; benchmarking

Both procedures are broadly distributed through participants. Participants use different models for the same issues and can be involved in cross-model verification or benchmarking, discussion on differences in uncertainties management in different repository development stages (end-points in uncertainty/sensitivity analysis, treatment of uncertainties in biosphere, data characterization (PDFs), etc.)

7.3.4 Operational safety

The specific risks or situations need to be addressed without any substantial feedback experience from the operation of existing nuclear facilities (management of concomitant activities, management of fire...). Parameters associated to the characterization of the considered risks (fire, flood...) needs to take into account the peculiarities of such a facility. Finally, the identification of Limits, Controls and Conditions for the operational phase remains a challenge, since it has to integrate the dimension of long term safety: the numerous links between pre- and post-closure arguments of the safety case call for a methodology to verify continuously that the operator is always on the right track to achieving its target, namely the conditions of the repository at the time of closure which form the basis of the demonstration that the facility is sure in the long term.

Needs for knowledge:

C4 A methodology to review the hazards possibly occurring in an underground nuclear facility and scientific basis associated to development of conventional/nuclear hazardous processes in underground

- fire hazard
 - o characterization of fires in underground spaces
 - thermal response of ILW emplacement cells on temperature rise aggressions
 - o quantification of effects of fire on specific target in confined environment
 - o integration of different confined environment in IRSN's simulation tools
- handling hazard
 - characterization of situations of stopping the transfer of canisters and emplacement
 - o consequences of these situation on the components relevant for safety and





on the general level of risks in the facility

- hazard due to activities performed in parallel (co-activity)
 - methods (including in other industries) for organizing safely activities performed in parallel
 - definition of situations (such as evacuation in the case of a fire in the underground area) that should be taken into account in the analysis of these risks

Currently available: expertise is available through the participants (see Table with models), however with some limitation and uncertainties (Geosaf II. Report).

Needed: It is necessary to addressed following issues

• operational hazards/safety issues specific to an underground nuclear facility (in terms of

large scale, difficult access, concurrent activities...)

• how hazards/safety issues are addressed in the operation of mines (conventional or uranium) or underground facilities (tunnels...) and in the operation of existing nuclear facilities

(including radioactive waste disposal facilities);

• the necessity of developing a specific safety approach for hazards/issues specific to an underground nuclear facility;

• the implications of these operational issues (including accidents) on post closure safety ;

• the recommendations with regard to the development and review of the safety case.

7.3.5 Monitoring

Identified R&D need for knowledge:

C5 To built confidence into monitoring methods in order to define the reference state of the system and its evolution during construction, operational and post-closure phases

Particular points of attention (not exhaustive list):

- The reference state is necessary to be known for comparison
- Monitoring confirms repository performance and verify the model predictions
- During construction phase: monitoring like for civil engineering/mining objects
- During operational phase: to confirm short term evolution and update the safety case; radioprotection
- During post-closure phase: until the end of institutional control

The issue is particularly country specific and monitored issue specific (dependent on regulator and legislation). There are 2 ways how to proceed:

- Evaluation of monitoring data, provided by implementer (need to understand to the data and purposes of monitoring)





- Independent monitoring

The basic step is to understand the monitoring methods.

Monitoring:

- Monitoring of overall state of the system (preliminary state, state during the construction, operation and post-closure state)
 - o Water
 - o Soil
 - o Air
 - o Radiation
 - Seismic (microseismicity)
- Issue-specific monitoring (dependent on host rock and DGR concept)
 - o radiation
 - o geomechanics
 - o massive stability
 - o water inflow
 - o water chemistry)

Possibly can be requested by the regulator.

8 Categorisation of scientific issues

The current R&D national programmes yielded by TSOs and regulatory bodies are of various level of maturity depending on the progress of the national disposal programmes. For this reason, it appears quite difficult to draw full common lessons and perspectives in terms of R&D joint programming regarding the various key questions identified. Maybe this objective could be envisaged by addressing two main categories of scientific issues: on the one hand those related to processes where the scientific community already made progress and where additional efforts concern specific ongoing development designs in selected sites (for more advanced programmes) - **specific issues**, on the other hand those related to generic scientific topics that concern any kind of programmes (more related to the assessment methodology).

Following topis are examples of those of more generic concerns

- Modelling coupled processes during transient phase (evolution of data...): the « movie » of the disposal
- Upscaling methods: from lab scale to site
- Accounting for uncertainties in scenarios
- Monitoring and measurement methods

Following topics are examples of those of more concept specific

- Waste matrix and source term: bitumen, glass fracturing, gas release, IRF





- Container: corrosion, μ-organisms, radiolysis
- Engineered components: geochemical interactions
- Host rock: methods to detect heterogeneities

However, collaborative programmes do remain of interest on some higher level scientific topics related to components and materials (behaviour of concrete, performance of seals...) or cross-cutting issues and integrated modelling (role of interfaces, coupling of processes for example, transient phase...).

The above mentioned R&D needs for knowledge were according to this conclusion categorised into either **generic concern topics (GCT)** or **concept specific ones (CST)**. Categorisation is important namely for identification modes of potential cooperation with other stakeholders. Basically, the stakeholders, namely WMOs, would appreciate cooperation namely on generic concern topics, stressing that governance for such activities is needed (see D3.3).

8.1 QUALITY OF INPUT DATA

8.1.1 Methodology adequacy and relevance

Identified R&D needs for knowledge:

A1 To assess the adequacy and relevancy of methods available for the evaluation of data necessary for long-term and operational safety demonstrations.

Particular points of attention (not exhaustive list):

-	Methods to characterize the source term	CST
-	Methods to characterize DGR thermal development	CST
-	Methods to characterize container corrosion rates	CST
-	Methods to characterize the geo-mechanical properties of the host-rock (ad coupled (T)HM behaviour)	vanced CST
-	Methods to characterize diffusion properties of the near-field materials and th rock	e host- CST
-	Methods to identify transport properties of the host rock (faults and joints)	CST
-	Methods for description of geological properties of the site	GCT
-	Methods to evaluate the sorption capacity of the near-field materials and the ho CST	st-rock
	Mathada to avaluate the normaphility of pear field materials and the best reak	<u>ст</u>

- Methods to evaluate the permeability of near-field materials and the host-rock CST

8.1.2 Representativeness of the evaluated data

Identified R&D needs for knowledge:

A2 To assess if the data evaluated at small scale (in time and space) are representative





for in situ repository conditions and future evolution.

Particular points of attention (not exhaustive list):

- Representativeness of rock properties (mineralogy and petrology, porosity, pore connectivity, fracturing, mechanical properties, thermal properties) GCT
- Representativeness of hydraulic performance of seals and concrete liners **GCT**
- Representativeness of the geological structures in 3D dimensions (e.g. seismic methods)
 GCT
- Representativeness of barriers transport properties (sorption, diffusion data, permeability) CST

8.2 UNDERSTANDING OF COMPLEX PROCESSES

8.2.1 Processes on which rest performances of individual components

8.2.1.1 WASTE FORMS

Identified R&D needs for knowledge:

- **B1** To develop independent understanding in the processes on which rest the performances of the waste form.
 - SNF disposal: characterization of the process responsible for the Instant Released Fraction (IRF) notably due to ¹²⁹I and ³⁶CI
 CST
 - Graphite bearing wastes (e.g. RBMK, UNGG reactor type): characterization of processes responsible for the ¹⁴C and ³⁶Cl release from waste forms **CST**
 - Vitrified waste: influence of the initial fracturing state of glass on its dissolution rate (and thus the radionuclide release rate) CST
 - The dissolution rate of the vitrified waste packages (e.g. influence high pH from the concrete environment) CST
 - Influence of dissolutions rates for radionuclide release from SNF (influence pH, Eh, oxidation/redox conditions)
 - Bituminised waste

8.2.1.2 CANISTER & OVERPACK

Identified R&D need for knowledge:

- **B2** To develop independent understanding in the processes on which rest the performances of the waste canister and its overpack.
 - The influence of the thermal dissipated power on the canister and overpack properties CST
 - The assessment of corrosion mechanisms and rates (e.g. generalised or pitting corrosion) in reference conditions **CST**

75

CST





- The dimensioning of the canister and overpack with respect to the different loads experienced under repository conditions (due to the host-rock behaviour and to the thermo-mechanical effects)
 The influence of corrosion layer on the extent of corrosion
- Influence of microbiota on corrosion rates CST

8.2.1.3 ENGINEERING BARRIERS (BUFFERS AND SEALS, CONSTRUCTION MATERIALS)

Identified R&D need for knowledge:

- **B3** To develop independent understanding in the processes on which rest the performances of the Engineered Barrier System (EBS).
 - Processes affecting the geo-mechanical properties of the EBS (swelling capacity of bentonite materials, change of the chemical composition of bentonite materials...)
 CST
 - Process affecting the hydraulic properties of the EBS (EBS permeability...) CST
 - Processes of buffer erosion (causing lost of the performance) CST
 - Processes on which rest the retention/sorption capacity of the EBS" CST
 - Interaction processes at the material border of materials (buffer/container; buffer/host rock)
 CST
 - Long term evolution of buffer and sealing materials (long term tests, natural analogues) CST

8.2.1.4 GEOSPHERE

Identified R&D need for knowledge:

- **B4** To develop independent understanding in the processes on which rest the performances of the Geosphere.
 - Long term stability of the geosphere (including seismic, orogenic properties) GCT
 - Processes affecting the mechanical properties of the geosphere and its healing (for clay rock and rock salt)
 CST
 - Influence of the mineralogical composition of the host rock on its sorption capacity. **CST**
 - The migration of radionuclides in the host-rock at ambient temperature and considering temperature gradient representative of those that may occur in the near-field of the foreseen waste disposal system
 GCT
 - Identification of fracture wetting surface in fractured rocks in order to determine the extent of radionuclide migration **CST**
 - Evaluation of indicators on the confinement capacity (i.e. diffusion dominated) at long-term, and its consistency with the DGR concept
 CST



Sustainable network of Independent Technical Expertise for Radioactive Waste Disposal



8.2.2 Processes resulting from internal and external perturbations

- Internal perturbations:

- Waste component/Host-rock and Waste/EBS interactions;
- EBS/Host-rock interactions;
- Perturbations during the operational phase;
- Perturbations due to constructions
- External perturbations.

8.2.2.1 INTERNAL PERTURBATIONS: WASTE COMPONENTS/HOST-ROCK AND WASTE/EBS INTERACTIONS

Identified R&D need for knowledge:

- **B5** To develop independent understanding in the internal perturbations of the disposal system resulting from the waste/host-rock and waste/EBS interactions.
 - Effects from waste forms:
 - The compatibility between bitumen waste and the surrounding concrete and host-rock (with respect to their potential swelling)
 CST
 - Generation of gases (H₂, O₂) upon radiolysis of pore water, microbiological degradation of organic-based waste (e.g. bitumen)
 CST
 - Radiation effects on materials
 - The gas issue
 - Gas release from waste packages and from the corrosion or radiolysis of engineered barriers
 CST
 - The study of the generation and migration of gas from the waste repository CST

8.2.2.2 INTERNAL PERTURBATIONS: EBS/HOST-ROCK INTERACTIONS

Identified R&D need for knowledge:

- **B6** To develop independent understanding in the internal perturbations of the disposal system resulting from the EBS/host-rock interactions.
 - Effects due to the corrosion phenomenon:
 - The corrosion behaviour of steel-based material in an anaerobic environment of deep repository
 - The clay materials evolution due to iron-clay interactions (characterisation and modelling)
 CST
 - Effect of interaction of bentonite/steel on corrosion layer development and influence on the corrosion rate
 CST
 - Anaerobic corrosion of iron metals is in addition connected with gas generation that can be detrimental to other components of a repository **CST**
 - Effects due to alkaline perturbation
 - The clay materials evolution due to cement-clay interactions by characterisation and modelling
 - Mineral transformations of bentonite in the alkaline front environment (it relates mainly to composition of penetrating alkaline waters, pH, single

CST

CST

CST

CST





CST

minerals transformation trend)

8.2.2.3 INTERNAL PERTURBATIONS DUE TO OPERATION AND CONSTRUCTION

Identified R&D need for knowledge:

B7 To develop independent understanding in the internal perturbations of the disposal system resulting from potential operational transients.

-	Effect of the oxidizing and desaturation transient process	GCT
-	Effects resulting from the presence of micro-organisms	GCT
-	Influence of defects, caused by handling, on canister corrosion	GCT

EDZ formation and extent

8.2.2.4 EXTERNAL PERTURBATIONS

Identified R&D need for knowledge:

- **B8** To develop independent understanding in the potential external perturbations of the disposal system.
 - General geological condition change (potential marine transgression, future permafrost/glaciations, site erosion, site seismicity, site uplift/subsidence) **GCT**
 - The changes of the properties of the natural and engineered barriers (through the changes in groundwater flow regime, chemical conditions) are strongly related to the condition changes which are expected in the future
 - Potential future human intrusion and activities (gas storage and extraction, geothermal energy, resources exploration etc.)
 GCT

8.3 VERIFICATION OF EXTENT, INTENSITY AND IMPACT OF PROCESSES

8.3.1 Reliability of FEPs and scenarios

Identified R&D need for knowledge:

- **C1** To evaluate the reliability of methodologies followed by the operators for the assessment calculations.
 - Features, events and processes that are potentially important for the safety of the disposal system should also be identified thus there is a priority suggested on the development of updated FEP databases. E.g.:
 - Safety functions of all system components should be developed for scenario development
 CST
 - FEP screening and scenario development should be supported by experimental demonstration and natural analogue observations CST

SITEX





8.3.2 Reliability of models

Identified R&D need for knowledge:

- **C2** To develop independent models in order to evaluate the extent, the intensity and impact of processes resulting from internal and external perturbations of the repository on human and the environment.
 - Relevance of underlying conceptual (phenomenological) models used for the performance assessment
 GCT
 - Investigate the influence of the level of abstraction and simplification (of mechanical, hydrological, thermal and chemical processes) on the results of the assessment calculations; so as the robustness of the data transfer from one system component to the other
 - Verification and validation of the models, both conceptual and mathematical ones **GCT**

8.3.3 Management of uncertainties

Identified R&D need for knowledge:

C3 To evaluate the methodology followed by operators for managing the uncertainties surrounding the safety assessments.

8.3.4 Operational safety

Identified R&D need for knowledge:

C4 A methodology to review the hazards possibly occurring in an underground nuclear facility and scientific basis associated to development of conventional/nuclear hazardeous processes in underground

8.3.5 Monitoring

Identified R&D need for knowledge:

C5 To built confidence into monitoring methods in order to define the reference state of the system and its evolution during construction, operational and post-closure phases

GCT

CST

GCT





9 Conclusions

The aim of Task 3.2 was to evaluate available facilities, equipment, models and capacities in order to cover R&D that would cover the needs for knowledge, identified in Task 3.1 [1]. Moreover, it was also aimed to identify needed/planned capacities and capabilities of individual TSOs and potential TSO's network.

Generally it is clear that some of the research areas are well covered (geochemical and geo-mechanical labs, modelling of transport and safety assessment etc.) Those are the topics, covering namely generic issues. Conversely, some of concept/site specific issues need to be either developed or the available resources are missing (study on bitumenised waste, influence of biota on corrosion, influence of defects etc.). However, the list of topics has been compiled on the basis of available resources of countries, participating in the WP3.

Basically, the number of installations and tools available decreases with increasing level of specificity for the scientific problem solved. High-level sophisticated installations and labs require advanced and comprehensive maintenance. Therefore not all institutions can effort to develop them and maintain them. The straightforward examples are radiochemical laboratories and underground labs as special facilities with specific rules. Moreover, some of the installations are missing at all, for example underground laboratories in crystalline rocks that are mostly owned or facilitated by the implementers (Grimsel, Äspö, Oikiluoto, Horonobe, etc.). Such installations should be either shared in case they are available within "independent" circle or joint projects with other institutions, including WMOs, should be launched. In the last case the governance on the joint research activities is requested.





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