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DISCO

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Kick-off minutes

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

Minutes of the Disco Project Kick-off meeting

13 June 2017, Brussels, Belgium

Time: 09.00 to ca 16.00

Location: The auditorium, BREY Building, European Commission

Address:

Breydel

avenue d'Auderghem, 45

1040 – Bruxelles

Invited: All participants, EUG including regulators & Christophe Davies.

For a list of participants, see attachment 2.

As the meeting location was changed to a new building, the start of the meeting was slightly delayed. After some technical assistance, Lena and Petra welcomed everyone to the meeting and showed the agenda. Below follows short notes from the different presentations. The presentations are distributed to the participants through email. It should be noted that the EC Project Officer is changed from Christophe Davies to Athanasios Petridis; however, Athanasios could unfortunately not attend, but the meeting was instead attended by Christophe Davies.

Euratom programme

The first item on the agenda was an overview of the Euratom funding scheme and funded projects in the Radioactive Waste area, by Christophe Davies, European Commission: "Status and Outlook of the Euratom Research & Training Programme (2014-2018) in Radioactive Waste Management".

This presentation included information concerning a report on the Waste Directive and the PINC Nuclear Illustrative Programme, both with aim to compile a comprehensive picture of the full costs linked to decommissioning and Waste management.

The current Euratom programme, 2014-2018, complements H2020. Christophe gave a background and overview of the Activity areas and current and planned Work Programme in Radioactive Waste Management. For the last call there were 13 proposals, resulting 5 funded projects: Disco (this project) , Beacon (bentonite project), Chance (waste characterisation), Insider (Site characterisation for waste minimization), and Theramin (Thermal treatment for waste).

In the future, the idea and hope is that "Joint Programming" should be implemented: the Joprad project is preparing the way for this. If successful, the European Joint Program should be initiated by mid-2019, and the Disco project would then be a part of the EJP.

Regarding project management and contractual obligations, the importance of communicating was emphasized. Projects are encouraged to use Twitter, and follow official account @EU_H2020. There is also a new hastag #ReserachImpactEU.

Not only articles and presentations need to acknowledge the Euratom funding but it is also required to mark equipment and experiments with need stickers acknowledging the Euratom funding.

Work package 1 Management, Coordination and Dissemination

An overview of the project plan and structure was given by Lena Z Evins and Petra Christensen, SKB (Coordinator), although this presentation was kept short due to the delayed start of the meeting. Gantt and Pert charts as well as WP1 deliverables were presented.

Work package 2 Preparation of samples and chemical systems

Next item on the agenda was a presentation of WP2 by WP2 leader Ian Farnan, University of Cambridge. The aim of WP2 is to ensure coherence between model systems and real systems, and to oversee chemistry of solutions. It includes three types of work: Hot cell work for real spent fuels, radiation protected laboratories for work with alpha doped materials, and U/Th gloveboxes for the work with UO₂ materials.

Four tasks are identified in this WP: Task1 : Hot cell. Here, work will be performed for the fuels that have not already been characterised in First Nuclides (KIT-INE, JRC, NNL). Task 2, alpha glove box (Jülich, SCK CEN, VTT, CEA) using pellet press & sintering Task 3 UO₂ : UCAM, USFD, Ciemat (pellet press & sintering) USFD will use hot isostatic pressing. Task 4: Coordination of aqueous solution chemistry in general three types of waters. In addition, real groundwaters from Finland will be used by VTT.

This WP starts at project start June 2017 and all work is foreseen to be performed by June 2019, and will deliver two reports: One describing the “initial state” for samples & experimental systems that will be used in dissolution experiments, and one describing the failed fuel from NNL.

Work package 3 Spent fuel dissolution experiments

The spent fuel dissolution work is collected in Work package 3, which was presented by WP3 Leader Ernesto González-Robles, KIT-INE. The partners performing spent fuel dissolution are: KIT-INE, JRC Karlsruhe, Studsvik and CTM (at JRC Karlsruhe).

The objective of the work package is to investigate the influence of the presence of dopants in the fuel, as well as influence of different environments (water composition, H₂ content). In addition, data regarding the instant release fraction (IRF) in those experiments performed with fresh samples will also be made available. A total of 12 leaching experiments, using UO₂ with additives (Cr, Al), MOX and standard UO₂, will be conducted and during a period between 2 and 3 years, January 2018 to January 2021.

Work package 4 Model materials dissolution experiments

After a coffee break, the WP4 Leader: Dirk Bosbach, FZJ, presented work planned for WP4. Partners contributing to WP 4 are : FZJ, SCK CEN, CEA, Ciemat, USFD, UCAM & VTT. The purpose of using model materials is to overcome the complexity of the real spent fuel. Using the carefully designed and characterised model materials prepared in WP2, the effects on dissolution behaviour of parameters such as microstructure, doping, reactive surface area, will be investigated. By determining the element release and corrosion rates for these materials, a link may be established between Spent fuel and model materials matrix dissolution behaviour.

The contributions of the different partners were presented. WP4 involves dissolution of materials doped with additives and alpha-emitting nuclides, in order to mimic ca 10 000 years old spent nuclear fuel. WP4 also includes “post-mortem” experiments to look at microstructure and reaction kinetics. As an in-kind contribution, materials mimicking ca 4000

and 40 000 year old fuel will also be made by SCK CEN. It is noted that USFD will contribute to this WP with an externally funded PhD student.

A specific mention on the sample radiation field: As a part of the sample characterisation, it is important to document the actual radiation field of the samples in terms of alpha, beta and gamma.

Work package 5 Chemical Modelling

WP5 was presented by Lara Duro, Amphos 21, WP5 Leader. The participants of WP5 are: Amphos 21, PSI, Armines and NNL.

Three tasks are identified in WP5:

1. Thermodynamic equilibrium calculations, both of the oxygen potential in the solids, and of dissolution/precipitation reactions inside the water-saturated canister.
2. Development of the Matrix dissolution model, incorporating redox and electron transfer reactions
3. MOX-matrix dissolution model, to study both effect of Pu content on the alpha-radiolytic dissolution kinetics and the interplay with Fe(II) species in solution.

These tasks will involve selection of data from thermodynamic databases and development of the solid solution model: this would describe the initial state of the solid before dissolution. The modelling of the dissolution process requires the inclusion of any potential secondary solids. In this WP, a conceptual model involving the metallic particles and the hydrogen effect will be developed and a reactive transport model will be implemented to simulate the dissolution. As in all modelling, it will be necessary to simplify the system, starting with a 1D system and if possible, moving to a 2D system. For the MOX in Cox water (French case), the previous reactive transport model will be developed further and include effect of iron corrosion products as well as radiolysis.

A specific mention (expressed by EUG) is that what we are hoping for is a clarification of the effect of three- and four valent additives (dopants).

WP1 Dissemination and Knowledge management

Lena Z Evins (WP 1 Leader) presented some of the tasks in WP1 which involved dissemination and exploitation, as well as training and knowledge management.

Related deliverables are: Web page (A21), Plan for Peer-reviewed papers (SKB), Newsletters (SKB), Webinars (A21/Plan with SKB), Mobility measures (A21/Plan with SKB), Meeting minutes & proceedings (A21), Linked-In Group (A21)

The web page address will be www.disco-h2020.eu and it will be managed by Amphos 21. It should be ready by M3 ie end of August. Webinars and Mobility measures, ie travel grants to meetings and short visits to JRC, are aimed at the members of the Associated group that are from countries with less advanced programmes (LAPs).

After this, the WP presentations were finished and the meeting took a lunch break.

Afternoon session

After a sandwich lunch, it was time for the afternoon session, which focused on an initial discussion concerning D5.1: “Agreement of conditions to consider in the models: discussions between modelling and experimentalists”. This was led by Lara Duro (A21) and Enzo Curti

(PSI). The following is based on notes from the discussion, by Lena Z Evins (SKB). It probably contains some misunderstandings and also is incomplete, but the aim is to convey the spirit of the discussion and some of the issues discussed.

First, the aims and needs of the WP5 partners were presented.

For thermodynamic modelling it is required to have as complete chemical composition of the materials as possible, that is, detailed tables showing elemental composition of the materials. This is also needed for any potential secondary solids. Regarding the aqueous solutions, the chemistry of the solution as a function of time is needed: not only the radionuclides but also the major elements and parameters.

The stoichiometry is important: this part of the modelling will provide a kind of initial state of the fuel sample. This would then be used as input for the second type of modelling.

Important data for the modelling of the dissolution process are volume/mass ratio, surface area (site density), information regarding the metallic particles (% of the surface area), solution composition, etc. Information concerning any change with time is relevant and important, for example the evolution of the chemical solution with time, for both major and minor elements. If possible, information concerning secondary precipitates should be transferred.

So, the modellers need to know: What will the experimentalists be able to deliver and when.

Some Issues that were brought up during the discussion are listed below.

*How to describe the metallic particles in the fuel: The size distribution is such that these particles are so small they cannot easily be imaged and therefore, it is hard to get data on the true size distribution or nr of particles per surface area unit.

*Solution composition. Carbonate under reducing composition & Young cement water. Also, the NNL situation is oxidizing. The young cement water is hard to model. Regarding the formation of colloids, it is important to use filtration and ultrafiltration.

*Use of hydrogen in experiments without metallic particles. It could be argued that this does not produce the reducing effect at the surface: however, there are hypotheses and data indicating that hydrogen does in fact have a reducing effect on a surface even without metallic particles. The general purpose is to mimic the conditions and processes inside a canister in the repository.

*Kinetic modelling, ie rate of change with time, vs. modelling the equilibrium, ie the state where no change is thermodynamically favoured: If you have a system where nothing changes, you will not get kinetic information. Discussion regarding if you model equilibrium or kinetics: are you modelling change with time or is nothing changing. However it should be remembered that the core of the problem is what is the fate of the oxidants produced by radiolysis. If nothing changes, if [U] does not increase, in a spent fuel or alpha doped system, it means something other than uranium is reducing the oxidants. Experiments will get both things changing with time and also some that do not change.

*The idea of a model: the model should predict an evolution. Thus, the model needs to consider the evolution of the oxidants and reductants.

*Temperature: the discussion needs to also involve temperature. The thermodynamic modelling of the oxygen potential in the fuel will consider high temperature. The second part of the modelling should be done at lower T: temperature extrapolation is a bit of a problem. 25 degrees will be used for the lower T since most data is available for that temperature. Increasing the T means increasing the uncertainty, because of the lack of data and need to extrapolate

*Radiolysis: we need to know the radiation field and yield of different oxidants in the different systems.

After this, the focus was turned more on the matrix prepared by WP5 (see Annex 1): this had been circulated before the meeting for the experimentalists to consider. The modellers need to know exactly what data the different methods mentioned in the GA actually will be delivered & available for the modellers to use.

Some examples of data: Estimation of the geometric surface area, both pellet & fragment; microstructural parameters, such as grain size & grain boundaries. It was noted that the identification and quantification of uncertainties are important. Give error bars! We need to include uncertainties.

It was decided that A21 should prepare a list of parameters, a “wish list”, for their modelling needs. This should preferably be done in an excel sheet, sent to every partner who will provide experimental data and when they expect to provide the data. The experimentalists will then fill in exactly what data they will deliver. This should be sent by email and a deadline should be given: around end of September.

Next meeting

Before the meeting was officially ended, it was suggested that the first Annual meeting could be held in the UK, most likely Sheffield, in May. The meeting would be held in conjunction with the next Spent Fuel Workshop, which University of Sheffield has volunteered to arrange. This would four days in May for both events, and the preliminary dates set were 7-10 May; however, it was later observed that there is a national holiday in Sweden on the 10 May (Ascension day). Therefore, the exact dates need to be further discussed.

End of meeting. The meeting ended with afternoon coffee.

Annex 1.

Preparatory work from WP5 for the Kick-off meeting of DISCO for discussion on the preparation of D5.1

In the following pages different matrices are presented, which are the result of crossing the information in WP2, WP3 and WP4 in the proposal. This is a draft document to be discussed during the afternoon session of the DISCO kick-off meeting to be held on the 13th June 2017 in Brussels.

The objectives are:

- to check that these are the experiments and the materials and conditions to use
- to discuss if and how the results are going to be considered in the models of WP5
- to open the discussion for the preparation of **D.5.1**. Agreement of conditions to consider in the models: discussions between modelling and experimentalists. Responsible: All partners. Due PM 6

Composition of the contacting solutions in the proposal:

Bicarbonate water: 1 to 2 10^{-2} M NaCl 1 to 2 10^{-3} M NaHCO ₃	Young cementitious water with Ca, YCWCa, pH ~13.5: Na: 1.4×10^{-1} M; K: 3.5×10^{-1} M; Ca: 4.8×10^{-4} M; Al: 6×10^{-5} M; Si: 3×10^{-4} M; SO ₄ ²⁻ : 2×10^{-3} M of SO ₄ ²⁻ , CO ₃ ²⁻ : 3×10^{-4} M	Synthetic CO _x water (Callovo-Oxfordian Water)
Reducing (H ₂), anoxic	Reducing (H ₂), anoxic	with and without Fe

Cross matrix WP2-WP3-WP5

WP2 Hot cell work

WP2 Hot cell work					Use in experiments WP3				WP5 USE IN MODELS
Fuel	Burn-up	Form	Characterisation	Partner	solution	redox	partner	nr. Tests	WP5 partner
MOX	38 GWd/THM	Two decladded fragments, one cladded segment (10mm).	Optical and electronic ceramography: grain-size, secondary phases and micro-cracking; gamma and Raman spectroscopy	KIT-INE	BW	reducing: Ar + 8% H ₂ ; 40 atm	KIT-INE	3	
MOX	40-60 GWd/THM	Cladded segment (2.5mm)	Optical and electronic ceramography: grain-size, secondary phases and micro-cracking; gamma spectroscopy	JRC	BW	anoxic: Ar	JRC	2	
Cr-doped	40-60 GWd/THM	Decladded fragments	Optical and electronic ceramography: grain-size, secondary phases and micro-cracking; gamma spectroscopy	JRC	BW	Reducing: 30bar H ₂ autoclave	JRC	1	

UOX	20-25 GWd/THM	Decladded fragments	Detailed characterisation of alteration products SEM, gamma spectroscopy	NNL					
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No correspondence with WP3 experiments in the case of the MOX to be characterised by NNL has been found. I do not know whether this implies that no dissolution tests will be done with this material or that I simply have not found them.

For some experiments in WP3 no characterisation of the corresponding solid in WP2 has been identified. I believe that the reason is that the solid comes from the First-Nuclides Project and was already characterised during it. They correspond to the experiments by Studsvik and CTM, the ones with a red square below (table taken from WP3 proposal).

Leachant	Conditions	Fuel	Burn-up (GWd/t _{HM})	# tests	Sample	Institution	Focus
Bicarbonate water (pH ≈ 8.3)	Anoxic	MOX	40-60	2	cladded segment (2.5 mm)	JRC	IRF and Matrix
	Reducing with the presence of dithionite as reductant agent in anoxic atmosphere	UO ₂	60	1	cladded segment (2.5 mm)	CTM	IRF and Matrix
	Reducing with the presence of H ₂ atmosphere	MOX	38	3	cladded segment (10 mm) and fragments	KIT-INE	IRF and Matrix
		UO ₂	57.1	1	decladded fragments	Studsvik	Matrix
		UO ₂ -Cr&Al doped	59.1	1	decladded fragments	Studsvik	Matrix
		UO ₂ -Cr doped	60	1	decladded fragments	JRC	Matrix
Young Cement water with Calcium (pH ≈ 13.5)	Oxidising, equilibrated with air	UO ₂	60	1	cladded segment (2.5mm)	CTM	IRF and Matrix
	Reducing with the presence of	UO ₂	60	1	cladded segment	CTM	IRF and Matrix

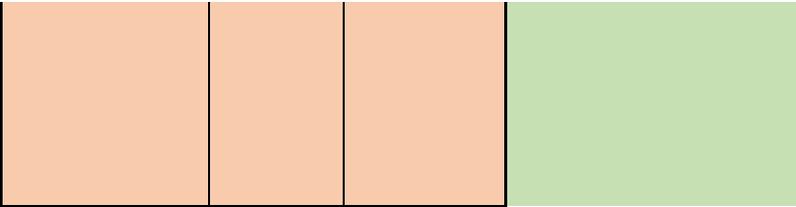
Cross matrix WP2-WP4-WP5

The same cross matrix but, in this case, for WP2-WP4-WP5. Two matrixes are included: one for alfa work and another one for inactive work.

WP2 α -glove box

WP2 α -glove box					Use in experiments WP4			WP5 USE IN MODELS
model solid	α -doping	simulation	characterisation	partner	solution	redox	WP4 partner	WP5 partner
UO ₂ ref	²³⁸ Pu/ ²³³ U	1e4 y	Alpha-enabled SEM, FIB and TOF-SIMS to take advantage of the model system approach.	. JUELICH . SCK-CEN . VTT	BW	H ₂	. JUELICH . SCK-CEN . VTT	
					YCWCa	H ₂	. JUELICH . SCK-CEN	
					Natural GW	Fe	. VTT	
UO ₂ + Cr/Al	²³⁸ Pu	1e4 y	Alpha-enabled SEM, FIB and TOF-SIMS to take advantage of the model system approach.	. JUELICH . SCK-CEN . VTT	BW	H ₂	. JUELICH . SCK-CEN . VTT	
					YCWCa	H ₂	. JUELICH . SCK-CEN	
					Natural GW	Fe	. VTT	
(Pu,U)O ₂ 25 wt% Pu	²³⁸ Pu ~ 2.2*10 ⁹ Bq/g		Samples already available will be annealed to restore stoichiometry, which will be checked with	CEA	COx		. CEA	

XRD and Raman
spectroscopy.



WP2 U-Th

WP2 U-Th				Use in experiments WP4			WP5 USE IN MODELS	
				solution	redox	WP4 partner	WP5 partner	
model solid	method	characterisation	partner					
UO ₂ reference	Hot-isostatic pressing	SEM, EBSD and XRD,	USFD	BW	H2	. JUELICH . SCK-CEN . USFD		
				YCWCa	H2	. JUELICH . SCK-CEN		
UO ₂ + Cr + Cr/Al	Hot-isostatic pressing	SEM, EBSD and XRD, selective area electron diffraction.	USFD	BW	H2	. JUELICH . SCK-CEN . CIEMAT . USFD		
				YCWCa	H2	. JUELICH . SCK-CEN . CIEMAT		
UO ₂ + Gd	Powder pressing & sintering	Raman, XRD, SEM, SIMS,	CIEMAT	BW	H2	. CIEMAT		
				YCWCa	H2	. CIEMAT		
UO ₂ +Cr	Powder pressing & sintering	Raman, XRD, SEM, SIMS,	CIEMAT					No dissolution test identified
U _{0.1} Th _{0.9} O ₂ and U _{0.9} Th _{0.1} O ₂	Homogenous nitrate synthesis	X-ray diffraction, SEM	UCAM	BW	H2			No dissolution test identified
				YCWCa	H2			No dissolution test identified
U _{0.1} Th _{0.9} O ₂ and U _{0.9} Th _{0.1} O ₂	Pressed & sintered from down blended U _{0.25} Th _{0.75} O ₂ (MELOX	X-ray diffraction, SEM	UCAM	BW	H2	. UCAM		

simulant)				
	YCWCa	H2	. UCAM	

As with experiments with fuel, there are some materials here where no experiments with the material have been identified (in yellow in the previous table) and the other way round, i.e., some tests indicated in WP4 with no identification of the solids that will be used (red squares in table below, table taken from WP4 proposal).

Samples	Bicarbonate water reducing, anoxic (H ₂) (derived from WP3) (+/- additional components)	Cementitious water (YCWCa) pH ~13.5, Reducing, anoxic (H ₂) (derived from WP3)	Synthetic COx water Callovo-Oxfordian Water) (+/- Fe(0))	Natural ground water, with Fe(0)
UO ₂ (reference sample) ¹⁾	JUELICH, SCK-CEN, USFD	JUELICH, SCK-CEN		
UO ₂ + α-dopant (Pu-238/U-233)	JUELICH, SCK-CEN, VTT	JUELICH, SCK-CEN		VTT
UO ₂ + Cr/Al ¹⁾	JUELICH, SCK-CEN, CIEMAT, USFD	JUELICH, SCK-CEN, CIEMAT		
UO ₂ + Gd ¹⁾	CIEMAT	CIEMAT		
UO ₂ + Cr/Al + α-dopant (Pu-238/U-233)	JUELICH, SCK-CEN, VTT	SCK-CEN, JUELICH		VTT
UO ₂ + Gd + α-dopant (Pu-238/U-233)	CIEMAT	CIEMAT		
Homogeneous unirradiated MOX (U _x Pu _{1-x} O ₂) (high α)			CEA	
MOX (U _x Th _{1-x} O ₂) ¹⁾	UCAM	UCAM		

Annex 2. Participants list.

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