

TRANSCEND (Transformative Science and Engineering for Nuclear Decommissioning) is a multidisciplinary collaboration of 11 universities and 8 key industry partners from across the UK's civil nuclear sector. Our world class £9.4M research programme comprises 40 projects which address some of the key challenges within the areas of nuclear decommissioning and waste management, with a special focus on the UK's needs. The work of the Consortium continues, rationalises and extends that previously DISTINCTIVE undertaken on (Decommissioning, Immobilisation and Storage Solutions for Nuclear Waste Inventories) with increased breadth, particularly in bringing together the academic and industrial communities to take more of a whole lifecycle approach to decommissioning and waste management.

It's now been 16 months since the programme started in October 2018 and we've been very busy during this time. We have held a Kick-off meeting, two Industry Road Shows, and our first Annual Meeting and set of Theme Meetings. Associated with the Annual Meeting we also held our first International Advisory Group meeting to allow their input to, and strategic leadership of, the Consortium's activities. We've been very busy recruiting post-doctoral researchers and PhD students, with the vast majority now in place so that technical projects are now well underway. Additionally, two of our academic members were seconded to BEIS for an extended period, allowing them the opportunity to gain policy experience and to use their expertise to provide input to relevant select committees and working groups.

There are also a number of exciting activities in the pipeline. Various TRANSCEND supported public outreach events will be held over the coming year through our participation in various Science Festivals, and we have also commissioned a public outreach activity regarding the social and ethical dimensions of waste management, based on workshops and interviews with both Consortium members and members of the public. We also have the production of a video about the Consortium planned, as well as a Public Engagement Summer School for all our researchers. I encourage you to regularly check our website (transcendconsortium. org) for updates on any upcoming activities.

The newsletter will summarise progress made by the Consortium in a digestible format. It will also contain key messages from our various management groups. Going forward, the newsletter will be published annually and will track the key outcomes and outputs during that period.

This edition focuses on previous

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meetings of the Consortium, and upcoming events. It also covers the experience of two of our academics who spent time at BEIS. Lastly, profiles for all the research projects underway and planned are included to encourage engagement not only by all Consortium members but also all stakeholders who have an interest in nuclear decommissioning and waste management.

I hope that you enjoy the first newsletter.

Mike Fairweather

(M.Fairweather@leeds.ac.uk)

TRANSCEND kicks off

Over 50 attendees gathered for the TRANSCEND kick-off meeting which was held on Wednesday 12th September 2018 at the National Railway Museum in York. The first part of the day was devoted to the research programme. Mike Fairweather (PI, University of Leeds) opened the meeting by presenting a general overview of the TRANSCEND project.

Presentations from each Theme Leader giving more detail on the planned research within their respective themes then followed. The morning was rounded off with a presentation by Joanna Renshaw outlining some of the proposed impact activities. Early afternoon saw the industry partners presenting details on their involvement with the project. The final part of the day was devoted to general discussions on projects and plans going forward.



Mike Angus (NNL) speaking about the benefits of TRANSCEND for industry.

TRANSCEND takes to the road

The TRANSCEND team took to the road in December 2018 and January 2019 to raise awareness of the consortium amongst the nuclear community. The 1st Industry Roadshow was held at Birchwood Park in Warrington on 11th December 2018 and the 2nd at The Mercure in Bristol on 14th January 2019. Nearly 90 delegates registered from organisations across the nuclear sector to attend the roadshows. They came to gain an overview of the research programme and to learn how it will help to address key challenges facing the industry. Both days started with Mike Fairweather (University of Leeds) giving a general outline of the project. Academic Theme leaders then presented further information on the research being carried out within our themes: Integrated Waste Management; Site Decommissioning & Remediation; Spent Fuels; Nuclear Materials. Finally it was the turn for the industry partners to speak about their involvement in the consortium. Both days provided fruitful exchanges between the academics leading the research and the industry stakeholders.



David Read outlines the plan for the Spent Fuels theme



Mike Fairweather talks about impact activities

1st Annual Meeting - Bath 2019

The consortium held its first annual meeting at the Apex City hotel in Bath on the 3rd and 4th April 2019. Over 100 representatives from academia, industry and government bodies gathered to learn about the latest research findings since the programme started in October 2018.

Sixteen technical presentations covered the 4 themes: Integrated Waste Management; Site Decommissioning & Remediation; Spent Fuels; Nuclear Materials.

Keynote presentations were delivered by Charlie Scales (National Nuclear Laboratory), Trevor Chambers (Imperial College, London), David Shoesmith (University of Western Ontario, Canada) and Helen Steele (Sellafield Ltd).

The posters displayed throughout the meeting generated a great deal of stimulating and thought-provoking discussion during the networking breaks.

During the final session of the meeting the audience learnt about linked programmes covering accident tolerant fuels (ATLANTIC - Accident Tolerant Fuels in Recycle), robotics and sensors for extreme environments.

The meeting dinner took place in the magnificent surroundings of the Roman Baths and Pump Room.



Pre-dinner drinks at the Roman Baths



Dinner in the Pump Room



Networking during the poster sessions

Theme Meetings - Lancaster 2019

The first set of Theme Meetings for TRANSCEND were held at Lancaster University Conference Centre on the 11th & 12th November 2019.

On day one, a combined agenda from Themes 1 & 2 included talks from experienced post-doctoral researchers, flash presentations from the PhDs as well as presentations from Ed Butcher and James Graham from NNL (the industry champions for the two themes).

On day two, parallel sessions from Themes 3 & 4 included presentations from TRANSCEND researchers as well as from researchers working on projects associated with TRANSCEND. Once again, industry champions from NNL - David Hambley and Robin Orr - had the opportunity to make presentations about the research programme from an industry perspective.

The thirty-six posters on show provided plenty of opportunities for researchers to engage directly with industry and other academic colleagues.







Save the Date

The 2nd Annual Meeting of the TRANSCEND Consortium will be held at The Majestic Hotel in Harrogate on 31st March and 1st April 2020.

Updates will be posted on the website -<u>transcendconsortium.org</u> and on Twitter -<u>@Transcend_epsrc</u>.

Please contact Dr Lois S Tovey (<u>I.tovey@leeds.ac.uk</u>) if you wish to be added to the mailing list for invitations.

Waste Management Symposia 2020, 8-12th March 2020, Phoenix, Arizona

The TRANSCEND consortium has its own dedicated session at WM2020 the leading international conference for the management of radioactive waste and related topics. Come along on the afternoon of Wednesday 11th March 2020 to hear about our latest findings and join us in our networking social after the presentations.

TRANSCEND Academics seconded to BEIS

The EPSRC TRANSCEND (Transformative Science and Engineering for Nuclear Decommissioning) project provides an opportunity for scientists to gain policy experience via funded secondments within Government departments. One of the first to undertake a secondment, Professor David Read, reflects on his experience of working part-time in the Department for Business, Energy, and Industrial Strategy (BEIS) over a period six months.

Prof Read is the NPL Professor of Radiochemistry at the University of Surrey and co-leader of TRANSCEND Theme 3 on Spent Fuels.

"In May 2019, I joined a team working on aspects of the Nuclear Sector Deal, specifically, nuclear decommissioning, waste management and geological disposal. It was an interesting time to join given rapidly changing events on the other side of Parliament Square. BEIS plays a major role in Brexit planning with many of its staff diverted to different tasks, often at very short notice. I was immediately impressed by the calmness of my new colleagues as they balanced urgent requests for information while maintaining focus on the much longer-term objectives of the nuclear sector.

My first task was to help draft a Consultation Document on radioactive waste management policy directed towards a more risk-informed approach, based on the radiological, chemical and physical properties of each waste stream. This is subject to public consultation but could potentially bring overall radioactive waste policy into line with that for low level radioactive, and other hazardous wastes, where the Waste Hierarchy and Proximity Principle are embedded. It could provide industry with greater flexibility in terms of management practices and encourage new entrants with opportunities for technology transfer. The proposals were at a fairly advanced stage when a decision was taken to broaden the remit and subsume the initiative into an overarching policy review covering nuclear decommissioning, radioactive substances and waste. As we speak, a public consultation is due to be issued around March 2020, though of course, a lot can happen between now and then.

My experience at BEIS has been extremely rewarding and given me new insight into how the Civil Service operates. The team I was assigned to was highly professional, inclusive, open to new ideas and made me feel welcome from the first day. As a scientist, I focussed my contributions on technical aspects, leaving policy communication to the experts; however, the scientific community and government agencies are working towards the same goals and better communication can only benefit both. I would thoroughly recommend others stepping across the line, if only for a short time".

(Disclaimer: the views and opinions presented in this post are those of the author and do not necessarily reflect those of the Department for Business, Energy, Industrial Strategy (BEIS).)



Pro Nuclear Demonstrators gather outside Parliament



Construction work at Hinkley C

TRANSCEND Academics seconded to BEIS

Laura Leay recently started a secondment to the government Department for Business, Energy and Industrial Strategy (BEIS). Her knowledge of analytical techniques that can be applied to radioactive waste can be shared with BEIS, providing expert advice that can be used to inform policy making.

At the start of her secondment, Laura spent a full week working in London and had a chance to meet the rest of the team at BEIS, attend a 'meet the ministers' session and join project meetings in Whitehall. Since then she's worked from her office in the Dalton Cumbrian Facility. The main project that Laura is involved in will provide updated guidelines on recovery in the event of a release of radioactivity into a public space. The project is a collaboration between BEIS, Defra, Public Health England and the Environment Agency and, as well as providing guidance on a remediation strategy, will also set-out which company or public body will be in charge at each stage of the recovery process. So far, she's looked at several software tools that can help estimate the volume of waste that remediation techniques could produce and is looking forward to the rest of the project which will investigate where the waste could be stored, and what the final fate of the waste would be.

Laura is also helping to organise a workshop to provide BEIS with the latest information on waste characterisation methods that are currently in development and could be applied to waste that might be generated during decommissioning of nuclear sites. This has relied on her network of contacts in industry and academia and will provide government with the latest information on technology that could change practises in waste management.

Overall, the secondment has provided Laura with a fresh perspective on the nuclear industry, building on her previous experience with NNL and Areva as well as her current research at the University of Manchester. She's keen to continue her involvement with BEIS and is looking forward to returning to London later in the secondment.



Dr Laura Leay outside BEIS





Department for Business, Energy & Industrial Strategy

New materials and methods for decontamination of effluent



Anthony Nearchou, PDRA, University of Birmingham

Aims

- To prepare and characterise new materials for uptake of 137Cs and 90Sr radionuclides from liquid waste streams.
- To improve the syntheses of these materials so they are more cost, energy and time-efficient for an industrial scale preparation.
- To assess the ion-exchange capabilities of these materials in the presence of competitive ions, different pHs, simulant solutions and under flow.
- To investigate alternative remediation techniques in particular the use of magnetic ion exchange materials that can be separated post-treatment via magnetism.

Progress

Successful synthesis of doped tin umbites at a reduced temperature – 150°C as opposed to 200°C.

Experiments are underway to evaluate the selectivity of doped tin umbites for 137Cs at low concentrations (ppm) in the presence of the competing ions K+, Na+, Mg2+ and Ca2+.

Currently working on constructing a magnetic separation rig to test and demonstrate the use of magnetic ion exchange materials for effluent decontamination.

Scoping studies of new ion-exchange materials



James Reed

PhD,

One of the key challenges in nuclear waste remediation is removal of caesium and strontium from effluent. Currently at the Sellafield site, natural clinoptilolite, from California, does this in a column process, treating 100's m3 of effluent per day. This clinoptilolite is of limited supply and may not be as effective at treating future waste streams. As a zeolite, clinoptilolite is resistant to radiation and cheap, as well as having a negatively charged framework capable of 'trapping' these radionuclides. An array of zeolites capable of selective radionuclide removal would help us meet future decontamination targets.

- Aims
- Discover what properties make the current source of clinoptilolite so effective.
- Investigate the ion-exchange performance of different, readily available zeolites in various effluents.
- Investigate pre-treatments that can improve the properties of existing materials. **Progress**

Have shown natural clinoptilolite can be readily desilicated and dealuminated. This could improve rate of ion-exchange and capacity of material.

University of Birmingham Demonstrated different levels of conversion of natural clinoptilolite to zeolite-P.

In-situ synchrotron X-ray diffraction studies of ion exchange in zeolites



Hannah Parish, PhD, University of Birmingham Porous materials are widespread in the nuclear industry due to their ability to take up radioactive cations such as Cs, Sr and I. Natural zeolites and related materials have also been used at the sites of nuclear disasters, for example Three Mile Island and Fukushima. Little research into the mechanism of the ion exchange process has been undertaken as of yet – an understanding of this and how it links to the material's properties would help to develop new ion exchange resins and also justify the use of naturally occurring materials for this purpose.

- Aims
- Gain an understanding of the mechanism of ion exchange in Mud Hills clinoptilolite, the material currently being used in Sellafield's SIXEP effluent treatment plant
- Look into alternative materials for Cs/Sr uptake from nuclear waste streams, e.g. the zeotype ETS-10
- Perform synchrotron studies (Bragg diffraction and Pair Distribution Function) to monitor the mechanisms of exchange and study the crystallography of these materials

Progress

Performed in-situ ion exchange experiments on beamline I11 at Diamond Light Source to monitor the Cs-exchange process in Mud Hills clinoptilolite

Analysed X-ray data obtained and have observed changes in the clinoptilolite unit cell, cation positions and cation occupancies

Particle-laden flow characterisation and prediction



Lee Mortimer, PDRA, University of Leeds

Aims

- Use high-fidelity immersed boundary method alongside DNS to study the effect that varying certain chemical and mechanical properties has on the resulting interaction dynamics and generate behavioural modification techniques.
- Use Lagrangian particle tracking techniques to study agglomeration in simple wallbounded turbulent flows and demonstrate effect of tweaking modification-capable system properties such as temperature, ionic strength and flow rates.
- Develop polymer laden flow simulation capabilities to determine the efficacy of promoting flocculation through polymer additives in waste slurry flows.

Progress

- Immersed boundary technique has been used to demonstrate the effect of modifying Hamaker constant, temperature, ionic strength and coefficient of restitution, the latter showing the greatest effect on controlling collision dynamics.
- Agglomeration has been studied in channel flows, with particles exhibiting increased tendency to agglomerate within the centre of the channel.

Simulation of complex particle flows



Bisrat Wolde PhD, University of Leeds

Nuclear energy plays an important role in providing reliable, low pollutant gas emissions such as carbon dioxide and affordable electricity. There are drawbacks on delivering this affordable energy future - the waste product of most nuclear energies are radioactive. Safely disposing of these radioactive contaminated materials requires expertise and it is an expensive process. Implementing scientifically robust, innovative approach to decommissioning and waste management is essential for legacy wastes as well as future nuclear sites. In this project a direct numerical simulation of particle flows will be implemented to understand the behaviour of Pond and Silo sludges.

Aims

- Modelling and simulating for Understanding Pond and Silo Sludge Behaviour
- The provision of a predictive capability to understand how sludges will behave is crucial to successful retrieval and completion of Post Operational Clean Out (POCO) operations
- Developing optimised single-phase circular pipe in turbulent flow at high Reynolds number using the direct numerical simulation (DNS)
- Develop and validate multiphase DNS in a horizontal and vertical pipe turbulent flow. Both
 polydispersed and irregular shaped particles will be tracked. Modelling and understanding
 pond and silo sludge behaviours behavioural modification techniques using first principles mathematical modelling
- Potentially, machine learning algorithms might be used to analyse the data generated during simulation such as neural network modelling

Simulations of Processes at and across Nanoparticle-Water Interfaces



Ella Schaefer, PhD, University of Manchester The irradiation of nanoparticles results in energy deposits, this can transport through them in various manners. If the nanoparticles are in aqueous environments, the transport of energy across the nanoparticle water interface can cause chemical changes in the surrounding water media. The chemical products of this energy transportation can be used as powerful anticancer agents, and thus has great relevance to healthcare applications. Similarly, the chemical changes can also lead to the production of hydrogen, understanding this would help support safe operations within the nuclear industry.

Aims

- Via a computational simulation, energy will be directly deposited into metal oxide/ hydroxide nanoparticles and into the surrounding water media; emulating the effects of radiation on sludges.
- The energy transfer across the nanoparticle-water barrier will be calculated and the resultant chemical changes will be modelled.
- It is hoped that the models and simulations will offer a greater understanding of processes at and across nanoparticle-water interfaces, and have a positive effect on both the healthcare and nuclear industries.

Progress

- A basic simulation method of depositing radiation into a nanoparticle and calculating the subsequent dose deposition has been developed using the TOPAS software.
- This will be run with various nanoparticles and radiation types.

Durability of Magnesium-Silicate-Hydrate Cements made from Brucite



The fuel ponds at Sellafield contain a brucite-rich sludge, with a pH of 9 - 10. The focus of the PhD is on storing the sludge and making it safe by converting the waste to a magnesium silicate hydrate (M-S-H) based binder.

Aims

The overall aim of the research is to determine how the sludge should be pre-treated to produce a suitable M-S-H based waste form and to characterise its long-term durability. This will be achieved via the following sub-objectives:

- Create artificial sludge like material by slow formation and sedimentation of Mg(OH)2
- Investigate cementation of artificial sludge by condition and mixing
- Process the simulated sludge to produce M-S-H based wasteforms
- Study the composition, microstructure, mechanical properties, volume stability and durability of the resulting M-S-H based wasteforms at different ages and conditioning regimes

Mercedes Baxter-Chinery, PhD, Imperial College, London

Progress

Compiled a database of experimental data and findings on composition, processing and properties of M-S-H

Begun experiments with mixing/casting of M-S-H mortar

Radiation effects on nuclear waste forms: How does the degree of crystallinity in a glass-ceramic affect radiation tolerance?



Tamas Zagyva PhD, University of Manchester

Ca/Zn borosilicate glass-ceramic material (containing durable powellite crystals (CaMoO4) in the glass matrix) will be used for the immobilization of radioisotopes in high-level nuclear wastes with high molybdenum content. The size of powellite crystals in the material varies due to the different cooling rates.

The different volume changes caused by the swelling of both the crystal and glass phases under irradiation could induce cracking in the nuclear waste. Cracking is undesirable for the long-term durability, therefore understanding the radi-

ation tolerance of Ca/Zn based glass-ceramics with different degree of crystallinity is crucial in determining their long-term performance.

Aims

- Irradiate Ca/Zn borosilicate glass-ceramic samples (with different crystallite sizes) to simulate the internal alpha radiation of the high-level nuclear waste.
- Use several analysis techniques for the characterization (e.g. scanning electron microscopy, X-ray diffraction, electron microprobe, Raman and electron paramagnetic resonance spectroscopy).
- Investigate the changes in the microstructure after the irradiation experiment (e.g. cracking, ion migration, precipitation of additional phases) and whether these changes decrease the long-term durability of the material or not.

Process Monitoring of Thermal Treatment of Radioactive Wastes



Alex Stone, PhD, Sheffield Hallam University Off-gas has been a consistent issue with radioactive waste thermal treatment; the environmental impact could be large and current ways of quantifying these gases are unreliable and not in real time. A new or novel way of monitoring these off-gases in real time could provide a valuable insight into the mechanics of melt evaporation and help understand the environmental impact of thermal treatment. We will also aim to reduce emissions by changing various conditions and components of the melt and control their expulsion into the biosphere. In particular, this study will consider real-time off-gas analysis and methods of reducing emissions, in the context of ILW thermal treatment.

Aims

- Develop a new novel system for the real time monitoring of radionuclides
- Validate on inactive and active sites
- Monitor the effect of changing melt conditions and components on emissions

Progress

- Literature review volatility of radionuclides in progress
- Benchmarking of current analysers in progress
- Training in glass preparation and analysis in progress

Understanding glass melt chemistry in thermal treatment of nuclear waste

Observing the chemistry of vitrification in terms of immobilising nuclear waste forms to better understand the chemical changes within certain glass types that make them more efficient, safe and economical when in usage as nuclear waste stores. Mainly focussed on waste loadings and volatiles rather than durability.

Aims

Lucas-Jay Woodbridge,

University of Sheffield

PhD,

- Understanding the effect that Barium has on a base MW borosilicate glass and its ability to waste load and immobilise
- Potentially look and the immobilisation of soda in POCO waste using titanosilicates
- Attempting to make crystalline silicotitanates into a glassy form in order to use its ion exchange capabilities in the immobilisation of Cs.

Progress

Made a base MW glass with Barium content successfully. Awaiting characterisation techniques before further work is done.

Use of colloidal silica grout for inhibiting airborne and waterborne radionuclide migration



Arianna Gea Pagano PDRA, University of Strathclyde Nuclear site decommissioning involves several stages, including waste retrieval, decontamination, deconstruction and remediation of the surrounding land. As decommissioning proceeds, there is a severe risk of radiation exposure due to the spread of radionuclides in groundwater, surface water and airborne particulates. Therefore, there is a need to develop soil/infrastructure grouting strategies, for application prior to and during decommissioning, that minimise airborne and waterborne hazard and environmental risk. Colloidal silica is a feasible grouting technology for application in nuclear decommissioning due to its ability to penetrate low permeability materials for hydraulic barrier formation, improved sorption capacity, structural repair and erosion inhibition. **Aims**

- Using colloidal silica grout to treat surface soils as a risk mitigation measure for inhibiting radionuclide migration
- Optimise sorption/desorption grout properties by addition of other materials (e.g. biominerals formed in-situ)
- Investigate the feasibility of in- and ex-situ vitrification/cementation of grouted soils, thus minimising waste volumes via redeployment of the silica as an integrcomponent of the final wasteform
- Repair of existing degraded cementitious waste packages

Electrokinetic remediation (EKR)



Jamie Purkis, PDRA, University of Southampton

Radionuclide contamination in the ground is a huge problem at nuclear plants. But how do we get it out? We can dig up and store the soil, but this doesn't actually reduce contamination, it just moves it. Plants, another possibility, are slow to grow. What we do, at Southampton, is electrocute soil to move ions (like 137Cs+) within chosen areas of the substrate (like a negatively charged cathode), minimising waste volumes. Electrokinetic remediation (literally, moving things with electricity) is an exciting technology to tackle radioactive contamination and we're scaling this up. EKR has already been used to remediate plutonium-containing soil at Aldermaston.

Aims

emerging sustainable remediation ideas and previous proof-of-concept work to develop novel ex-situ and in-situ low-energy electrokinetic based remediation, stabilisation or clean-up approaches for complex site materials at working (and legacy) nuclear sites In-situ groundwater monitoring to improve identification of ground/ soil contamination volumes and associated contamination in ground infrastructure that may remain at the Site End State



It is of great importance to assess underlying soil surrounding nuclear facilitiesprincipally to detectpotentially hazardous substances that might be released to the environment.Standard methodsto monitor these contaminantswithin the groundwater floware mainlythrough samplingfrom boreholes and furtherl aboratory analysis. Additionally,in-situ measurements can be done through portable systemsthat comprise a probedeployed in a borehole on a push rod cable. This a fast, robust and reliable technique however is not suitable to be left in harsh environmental conditionsfor long-term, haspoor spectroscopy and might not be suitable for high radiation measurements.

Aims

- Rapid identification of hazard radionuclides in underlying soil and groundwater.
- Reduction of the need to human intervention thus reducing the radiation exposure to workers.

Objectives

- Develop a resilient device to be left in-situ for long-term down-hole monitoring.
- The system shall yield a degree of spectroscopy to identify principally Cs-137 and potentially Sr-90.

I am using gamma spectroscopy to identify the contents of buried, radioactively contaminated pipes and other underground structures. Once this has been achieved, I will be developing **Predicting Gamma** a non-invasive, geophysical technique to determine the dose rate as a function of depth and **Dose Rates with** shielding, incorporating environmental factors such as soil moisture content, structure type, **Limited Information** extent of contamination (point versus dispersed) etc. Aims Identify the contents of underground pipes and other buried structures using gamma . spectroscopy Use Geant4 to model buried pipes, continually comparing the model results to representative laboratory trials and field tests Develop and conduct lab-based experiments to understand the impact of environmental factors and shielding on the activity measured. Develop a smart algorithm combining the available diagnostics to calculate dose rate as a function of depth Develop and apply the algorithm to create a general methodology to transfer the process on a range of contaminated underground structures. **Progress** Luke Lee-Brewin A review of relevant literature has begun, covering waste handling regulations, gamma detection and peak analysis. PhD, Development of a laboratory experiment is underway. University of Surrey Discussions have been held with Magnox regarding access to a site for results verification. This PhD project aims to develop a new biomineral concrete repair strategy Assessing Degraded concrete samples taken from Davenport, Plymouth, will be repaired the strength and then tested for shear and unconfined compressive strength. The results will of biomineral be compared with more traditional repair techniques in the laboratory. The main strategies for target of the project will be to develop a model that simulates both the repair and subsequent failure of the samples. This model will then be used to improve the concrete repairs design of the repair strategy and to provide information for field trials which will be conducted in year-3 of the PhD. This project will be focused on Microbially Induced Carbonate Precipitate (MICP) via urea hydrolysis. MICP has been proposed for a number of engineering

via urea hydrolysis. MICP has been proposed for a number of engineering problems such as soil strengthening, permeability reduction, sealing fractured rock and more. No research has yet modelled MICP repaired concrete. Such a model will help to identify key controls on the mechanical behavior of treated concrete and can be used to develop improved treatment strategies. Modelling will be at the mesoscale level (mm-cm) and will explore the behavior of composite concrete/ calcite materials under various loading conditions within a Finite Elements Modelling (FEM) Framework.

Soraia Elisio, PhD, Lancaster University

Than



Assessing the properties and release behaviour of products arising from metallic and exotic fuel corrosion.



The current project aims to shed some light on the corrosion behaviour of metallic uranium in a wide range of environments, including water, uranic and Magnox sludges. Experimental work includes the preparation of small scale trials which are being investigated at distinct time interval using predominantly X-ray tomography.

Aims

- Determining uranium corrosion rates at ambient conditions
- Determining uranium corrosion morphology
- Investigating the identity of the arising corrosion products.

Progress

Corrosion percentage/rates over time has been already determined for a considerable time period

Haris Paraskevoulakos, PDRA, University of Bristol

An Investigation of Corrosion and Leaching of Carbide Fuels in a Geological Disposal Facility (GDF) Setting



Dimitris Samaras, PhD University of Bristol

The Safe Disposal of Advanced Nuclear Fuels



Ian Robertson, PhD, Lancaster University Uranium Carbide is an exotic fuel, and the legacy of the early UK Nuclear Research Programme. It was used in reactors such as Dounreay, and as an accelerator target in facilities like CERN. The NDA has accumulated a large quantity of this fuel, with disposal in a geological disposal facility (GDF) being its ultimate fate. Uranium Carbide is highly reactive with water and oxygen, with the potential for pyrophoric behaviour; both corrosive agents will be present in the environment of a disposal facility. The probability of interaction between groundwater and the carbide fuels is very high, which renders studying this interaction vital; in this PhD, groundwater environment will be simulated through the use of special cells, along with material and chemistry analysis to understand material change through exposure to water. **Aims**

- Pre-Corrosion Material Analysis: X-Ray Diffraction & Fluorescence, High Speed Atomic Force Microscopy, Scanning Electron Microscopy. Water immersion in special experimental cells.
- Gas Evolution Analysis: Residual Gas Analysis.
- Corrosion Material Analysis: aforementioned techniques, with the addition of
- X-Ray Tomography, Electron Microscopy, and Secondary Ion Mass Spectrometry Solution Analysis: Inductively Coupled Plasma Mass Spectrometry and Optical Emission Spectrometry, and Time Resolved Light Fluorescence Spectrometry

The aim of the current PhD project will be to develop and characterise a realistic MOX spent fuel simulant and use it to investigate the corrosion/leaching behaviour of MOX spent fuel under conditions analogous to those found in a GDF both (i) pre-closure and (ii) post-closure (oxic and anoxic conditions respectively). **Aims**

- Production and characterisation of simulated unused MOX fuels to serve as baseline systems.
- Production and characterisation of simulated used MOX fuels..
- Solution phase electrochemical corrosion and leaching behaviour studies of MOX simulants, aiming to obtain fuel dissolution rates as a function of key variables such as pH, salinity, O2 availability and temperature.
- Facilitated by collaboration with NNL, to assess how closely the simulants represent the physico-chemical and materials properties of real spent fuel.
- Progress

Literature Survey/Review commenced.

Identified CeO2 (Ceria) as a PuO2 surrogate.

Currently preparing to produce first pure CeO2 pellet and mounting to make an electrode for electrochemical corrosion studies.

Designing matrix of experiments to be performed.

Predicting the Alteration of Spent Nuclear Fuels	Ensuring the safe surface storage of spent nuclear fuel (SNF) over short-term and long-term timescales is difficult. There is significant uncertainty around the alteration and mobilisation of uranium within SNF pools and silos. The alteration products are expected to be similar to naturally occurring uranium minerals, of which more than 250 are known to exist. Understanding the alteration and transportation mechanisms of SNF is key towards providing solutions for the safe storage and disposal of SNF
	 This work aims to predict the alteration mechanisms and products of SNF. Real time, in situ spectral characterisation and computational modelling of SNF analogues and identification of their alteration products performed under different key environmental conditions (e.g. water, saltwater and water with hydrogen peroxide). Experimental characterisation and computational modelling of possible interference from known alteration of Magnox alloys, brucite (Mg(OH)2). Progress
	Experimental characterisation and computational modelling of the Raman and IR spectra of - brucite.
Joshua Bright,	Time Resolved Laser Fluorescence Spectroscopy (TRLFS) data obtained for hydrogen peroxide
University of Surrey	Experimental Raman and TRLFS spectra obtained for a selection of uranyl oxide hydrates.
	Multi Scale modelling using COMSOL/EACSIMILIE elengside testing the MOOSE Einite
A Predictive Tool for Spent Fuel Behaviour	Element framework to predict the behaviour of spent nuclear fuel (SNF) in multiple disposal scenarios. The models will be used to test alongside experiments to better understand scenarios such as failed waste inside legacy ponds to exposed UO2 in a long-term Geological Disposal Facility (GDF).
	 Aims & Objectives Build an improved Radiolysis model incorporating effects from geometrical considerations to H2O2 and H2 profile from the interface
	 Incorporate radiolysis model to a suspended particle dissolution model Predict chemical behaviour of suspended particles of SNF in legacy fuel pond storage Create a comprehensive 2D dissolution model of UO2 in multiple scenarios Design and test a Uranium particle dissolution experiment to test surface area to volume effects on rates of dissolution Implement work done on UO2 single and polycrystalline thin films to investigate grain size
	effects on dissolution rates _ Progress
Angus Siberry PDRA,	Successfully implemented a model based on work by L Wu (2014) of a 1D chemical reaction and diffusion model in COMSOL Investigated the effects of alpha particle dose rate and dissolution rate in an interim storage dose
University of Bristol	regime
Contact Angle Measurements and Wettability of PuO2 surfaces	About 140 tonnes of Pu are stored at the UK Sellafield site alone, the product of approximately 50 year's civil nuclear fuel reprocessing. The high radioactivity and half-life of these Pu-containing waste-forms necessitate intermediate storage, followed by recycling as mixed-oxide fuels or long-term disposal in a geological repository. Pu waste is generally stored as calcined plutonium oxide powders. Although typically sealed against environmental water ingress, the atmosphere may contain significant amounts of water. It is therefore essential to understand the behaviour of plutonium oxide under storage conditions, particularly in the presence of water, so ensure any interactions over time do not compromise the integrity of the storage systems used.
	AimsDevelop method of depositing thin-films of PuO2 and PuO2-structural analogue surfaces, particularly CeO2 and ThO2.Design and build an imaging system capable of visualising thin-film surfaces under controlled humidity. Measure the contact angle of water droplets on PuO2 analogue surfaces at a range of humidities and calcination temperatures.Subject PuO2 analogue surfaces to alpha particle bombardment to simulate aging of radioactive material. Measure the contact angle of water droplets on the aged surfaces Calculate surface-roughness and wettability factors, and determine the effect of radioactive aging.Procress
Dominic Laventine, PDRA,	Thin-films of CeO2 and ThO2 have been produced on glass and metal (Al,Ti) substrates. Prototype imaging system built and initial contact angle measurements taken at a range of humidities and
Lancaster University	Calculations of alpha particle energies to produce different amounts of damage, and discussion with DCF to organise use of the ion beam there.

Characterisation of AGR Fuel and its Behaviour During Drying



Thomas Bainbridge, PhD, University of Leeds

The UK's current plan is to wet store spent AGR fuel until a geological disposal facility is available to be used. Current experience of storing AGR fuel covers 20 years however it is expected to be 2075 before the GDF is available. Therefore an alternative storage solution is needed should an issue arise during wet storage which occurs in the time beyond our current experience of wet storage. Before the fuel can be disposed of in a GDF it will need to be dried to reduce the risk of hydrogen build-up.

Aims & Objectives

- To prove that cracked Advanced Gas-Cooled Reactor (AGR) fuel can take on water and be dried.
- To crack stainless steel in a representative way.
- To remove all the required water through the cracks produced.
- To estimate the flow rate through the cracks
- To develop a process model which is capable of predicting the removal of water from a cracked pin.

Progress

To date I have mainly been researching methods that could be used to produce stress corrosion style cracks in stainless steels including the Huey test as well as drop evaporation testing. I have also been spending time using a drying rig developed during a previous PhD to try and recreate results obtained there as a way to get myself used to operating it.

Development of Micromechanical Testing Methods for Spent AGR Cladding to Examine Effects of Sensitisation and Stress Corrosion Cracking



Kuo Yuan PhD, University of Bristol

In-situ Identification of Surface Corrosion Products on Spent Nuclear Fuels



Victoria Frankland, PDRA, University of Surrey Advanced gas-cooled reactor (AGR) spent fuel cladding is stored in spent fuel ponds and, over time, the cladding can suffer from stress corrosion cracking (SCC) induced from sensitisation by irradiation. A better understanding of the SCC behaviours and the change of mechanical properties of the material is required. In this research, digital image correlation will be implemented, and a new SCC sample set-up will be designed. **Aims & Objectives**

- The overall aim is to better understand SCC (including initiation), the change in the mechanical properties, and to develop new testing methods.
- State-of-the-art techniques to investigate SCC will be evaluated
- Relatively large samples with a large number of grains will be tested using full field DIC to study the initiation of SCC
- New testing set-ups will be designed with a smaller sample size while keeping relatively complete features of the bulk materials
- The materials will be modelled at multiple scales, and crystal plasticity will be introduced to study cracking at grain level

Progress

Previous studies of the topic, and state-of-the-art techniques have been reviewed Training has been undertaken on DIC operation

20/25/Nb AGR fuel cladding sample material has been obtained from the National Nuclear Laboratory

Presented poster at TRANSCEND Theme meeting in Lancaster, November 2019

Monitoring the corrosion behaviour of spent nuclear fuels (SNFs) is required to ensure safety and to inform decisions on future treatment and disposal options. It is possible that this can be achieved using remotely operated techniques, including the laser-base methods of Raman, time-resolved laser fluorescence (TRLFS) and laser-induced breakdown (LIBS) spectroscopy. Characterisation of natural uranium minerals, representing potential corrosion species, provides essential reference spectra for identification and purposes whereas real-time corrosion experimental simulation of the corrosion process(es) on thin film surrogates will help validate models of reaction pathways and kinetics.

Aims & Objectives

- Characterise a large range of uranium-bearing minerals, analytical grade uranium compounds and uranium-bearing solutions by laser fluorescence, Raman and laser-induced breakdown spectroscopy.
- Build database of characterised uranium phases.

Progress

Successful characterisation of a selection of uranium bearing minerals (loaned from the British Geological Survey and the National Museum of Wales) and uranium-bearing compounds (Universities of Surrey and Sheffield).

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Atomistic simulation of Am incorporation into PuO₂



William Nielson, PhD, Lancaster University

Since sealing, some canisters exhibit signs of becoming pressurised. A possible explanation is the evolution of hydrogen gas from corrosion of the surface by entrained water. The conditions do not appear to be sufficiently oxidising to promote corrosion, however studies have indicated the existence of a hyperstoichiometric PuO2+x that could act as the precursor to corrosion. Oxidation may be being driven by changes in the defect chemistry of PuO2 due to radioactive decay, in particular, the accumulation of americium.

Aims & Objectives

This project will use atomistic simulation to understand the defect chemistry of PuO2, and look at if incorporation of Am into PuO2 may contribute to canister pressurisation. Will first predict defect chemistry in pure PuO2 as function of environmental variables. Will next determine the energies of americium incorporation for all possible oxidation states, allowing prediction of: the mode of Am incorporation, its oxidation state and the presence of charge compensating defects.

Progress

Project at infant stages but have begun to investigate ability of Cooper Rushton Grimes potential to replicate experimental PuO2 data. Phonon density of states, lattice parameters & elastic constants of PuO2 have so far been examined.

Quantum chemical calculations (DFT), in the periodic boundary condition (PBC) framework,

Non and dissociative adsorption of water on stoichiometric and substoichiometric ThO2

surfaces - comparison with our previous work on water adsorption on other AnO2 (An =

substoichiometric ThO2 surfaces, in the presence and absence of water. Extension to PuO2. Surface chemistry of other small molecule species (NOx, ozone) on stoichiometric and substoichiometric ThO2 surfaces, in the presence and absence of water. Extension to PuO2.

Surface chemistry of water radiolysis products (HO· and H·) on stoichiometric and

Quantum chemical modelling of PuO₂ surface chemistry

Xiaoyu Han PDRA University of Manchester

Aims & Objectives

will be employed to study:

- Understand the surface chemistry of the ThO2. Extension to PuO2. Study the ThO2 surfaces interaction with water and the water splitting reaction pathway. And the full free energy of the reaction pathway will be delivered. Extension to PuO2.
- Other small molecules reaction with surface of the ThO2.

Progress

U-Cm).

- Benchmark the computational settings on the ThO2.
- The computational XRD reveal the interested facets including low index (001), (110) and (111), as well as the high index (311).
- The single water molecule adsorption on the ThO2 (111) surface.

Gas Generation from the Radiolysis of Water on Uranium and Thorium **Oxides**



Chris Anderson, PhD, University of Manchester Interactions between radiation and water is known to produce several products both stable and reactive. The production of hydrogen as one of the final stable products is particularly concerning for plutonium storage at the Sellafield site, potentially having ramifications for storage integrity. Water adsorbed to a metal-oxide interface is known to heavily influence the radiolytic hydrogen yield. While the use of uranium as an interface has been shown to increase the yield, thorium has yet to be explored in this context and may prove useful for predicting the radiochemical properties of plutonium during storage.

Aims & Objectives

- Determine the yield of gas (mainly hydrogen) produced from water adsorbed to UO2 and ThO2 surfaces after undergoing irradiation.
- Ascertain the of hydrogen yield when modifying variables such as RH% and sample mass
- Model the hydrogen-water-oxide interactions during irradiation.
- Assess the suitability of ThO2 to act as a PuO2 surrogate

of the ageing of PuO₂

Elanor Murray, PhD, University of Birmingham •

Atomistic Simulation The UK has the largest civil stockpile of plutonium in the world, stored at Sellafield. However, ageing mechanisms associated with the storage of PuO2 are poorly understood. The generation, stability and mobility of fission products, in addition to the role of the surface oxide layer are key factors. Atomistic simulation techniques are ideally suited to provide fundamental insight into the defect chemistry of PuO2, in order to further understand ageing phenomena.

Aims & Objectives

- Simulate defects in bulk PuO2 to identify which are likely to occur.
- Simulate pure and defective surface structures, investigating extended defects such as grain boundaries.
- Model helium incorporation within PuO2, and investigate helium migration pathways.

Progress

- Simulated intrinsic defects in bulk PuO2, found schottky trios and oxygen Frenkel pairs to be the most energetically favourable.
- Begun simulating pure surfaces, found 111 to be the most stable.

Underpinning plutonium immobilization in advanced ceramics wasteforms



Shikuan Sun

PDRA, University of Sheffield

Disposability of wasteforms for plutonium immobilisation and efficacy of surrogates



Clemence Gausse, PDRA, University of Sheffield Immobilizing plutonium wastes in ceramic will reduce the overall volume for geological disposal in the future, which will save on volume and cost.

Cold-press sintering can be firstly used to prepare zirconolite ceramic wasteform, contributing to the processing parameter selection, the formulation optimisation (loading, target site and charge compensator) and the understanding of the long-term stability. Such results will provide the guidance on the following hot isostatic pressing to process the advanced Pubearing zirconolite wasteforms.

Aims & Objectives

- Understand the crystal feature of zirconolite against the waste-loading and the existence of secondary phase.
 - Optimise the waste loading and formulation.
- Understand the long-term stability (dissolution & radiation) of Pu-substituted zirconolite. **Progress**
- Optimisation studies have been performed in developing zirconolite ceramics wasteforms.
- The local environment of Pu surrogate and the charge compensator was investigated in details.
- Now the project aims to develop an understanding of wasteloading with respect to advanced ceramics wasteform concepts, through a series of preparation-analysis experiments.

A small portion of the 140 tons of UK civil Plutonium stockpile has been considered as unsuitable for reuse as fuel. Zirconolite glass-ceramics, produced by Hot Isostatic Pressing (HIP), were selected as a promising immobilisation matrices for these so-called plutonium residues. Recent work by the University of Sheffield has shown, for materials using U and Ce as a surrogate for Pu, that zirconolite glass-ceramics exhibit good radiation stability, however, the aqueous durability of these materials in a geological disposal facility is not understood. An understanding of the efficacy of using Ce, Th and U as surrogates for Pu during durability studies is also required. Aims

We aim to resolve the key uncertainties pertaining to zirconolite ceramic/glass-ceramic dissolution in support of RWM S&T plan. The key objectives are to:

Understand the effects of relevant geochemical parameters on the kinetics and mechanisms of dissolution of HIP-ed ceramic/glass-ceramic zirconolite materials, using Ce and U as surrogates for Pu, and provide an assessment of representative leaching rates;

Perform selected experiments to understand the dissolution of 239Pu-doped ceramic/glass-ceramics, to understand the effect of solution radiolysis on the dissolution rate of glass-ceramics, in comparison to surrogate materials;

Establish a series of long-term (1 - 3y) dissolution experiments with 239Pu-doped samples, to inform the design of a future work programme to understand the fundamental material dissolution rates. Progress

Previous research (S. Thornber - DISTINCTIVE project) has shown that the microstructure and the partitioning of Pu in zirconolite ceramics/glass-ceramics, synthesised by HIP, is the same as the Ce and U surrogate samples. Further samples are currently being synthesised (using Ce and U) for initial dissolution studies.

Radiation Induced Changes in Effluents/Sludges



Mel O'Leary PDRA, University of Manchester

This project investigates radiation-induced processes involving Magnox nuclear waste sludges, which are poorly characterised; this project attempts to expose the underlying mechanisms at work in the sludges to inform their current and future handling. The processes involving the breakdown through irradiation of the sludge constituents to produce hydrogen are being investigated. In the sludges radiation is an effect of radioactive material in sludges. This project irradiated, with x-rays, simple materials which mimic the properties of sludges to investigate these mechanisms. The two properties have been measured are the effective hydrogen diffusivity in the sludge mimic and the radiolytic yield of hydrogen in the sludge mimic (the G-value). The effective hydrogen diffusivity is bounded by a simple geometric model. The radiolytic yield is accounted for with a model of radiation transfer mechanism. These properties have been used to predict the radiolytic production of hydrogen bubbles.

Characterisation of thermal treatment products



Daniel Parkes PhD, University of Sheffield

Contaminated mercury is a problematic orphan waste arising across the NDA, LLWR, AWE and MOD estates. EU restrictions on mercury import / export mean that there is an excess of market supply, which is a barrier to decontamination and reuse; the alternative is conditioning for disposal. The aim of this project is to develop a simple one-pot process for conversion of contaminated mercury to cinnabar and encapsulation in a phosphate cement matrix. The objectives are to demonstrate: 1) An efficient process for conversion of Hg metal to HgS, via phosphoric acid digestion and sulphide precipitation; 2) An optimised cement formulation to achieve one pot encapsulation of HgS in a phosphate cement, with no secondary waste generation; 3) The acceptability of the wasteform for storage and disposal. This approach will be developed alongside an evaluation of conventional OPC encapsulation and potential high temperature alternatives.

Building the foundations of a predictive tool for spent fuel behaviour



Jacek Wasik, PDRA, University of Bristol

The overall aim of the project is to construct the basis for a predictive tool for spent fuel behaviour; to model spent fuel in aqueous environments, across length-scales, using results from atomistic simulations, using physical and chemical kinetics, combining radiolysis models with molecular dynamics. We plan to close the loop between experiment and theory, by designing experiments that mimic and test the idealized scenarios implicit in these models. This project will bring the theorists and experimentalists together on a joint venture; retaining, building and developing knowledge-base for future generations.

Later, we plan to increase the complexity of the model; adding defect impurities, lattice damage, modifying the crystallography and the stoichiometry. We plan to vary the physical and chemical environment; mimicking the fuel in the spent fuel pool, in long-term storage and in operation, during an accident scenario. In the longer term, this approach will be extended to exotic fuels (nitrides, silicides for example), linking to work in the ATLANTIC consortium.

Conditioning and encapsulation of mercury contaminated



To be recruited, PhD, University of Sheffield

Contaminated mercury is a problematic orphan waste arising across the NDA, LLWR, AWE and MOD estates. EU restrictions on mercury import / export mean that there is an excess of market supply, which is a barrier to decontamination and reuse; the alternative is conditioning for disposal. The aim of this project is to develop a simple one-pot process for conversion of contaminated mercury to cinnabar and encapsulation in a phosphate cement matrix.

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Novel approaches to encapsulation of low level waste



Achieving passive safety for the radioactively contaminated materials produced during decommissioning is paramount for the long term above-ground storage envisaged. Much of the waste arising from decommissioning operations is still to be treated, and a significant portion of this is incompatible with existing solutions. Advanced treatment methods, such as thermal treatment, offer significant volume (and hence cost) reduction, but are technologically immature and the waste products require further underpinning before deployment at higher TRLs. This WP will assess the potential of magnesium-based cements as an encapsulant.

To be recruited PhD, University of Strathclyde

Electrokinetic remediation application to soils, concretes and other site and process wastes (including EDTAcontaining wastes)



To be recruited, PhD, University of Southampton

Despite a range of existing soil and water remediation, and waste clean-up, techniques available to nuclear site managers, effective in-situ and ex-situ remediation remain a common technical challenge, particularly at sites with complex or low permeability soils / subsurface geology, and on working sites or sites with considerable surface and subsurface infrastructure. This research builds on emerging sustainable remediation ideas and previous proof-of-concept work at the AWE Aldermaston site to develop novel ex-situ and in-situ low-energy electrokinetic based approaches that can be flexibly applied to different site materials and work around existing site infrastructure, providing new and flexible approaches for complex site materials (including low-permeability soils) at working (and legacy) nuclear sites.

Muon Tomography for Monitoring Civil Nuclear Assets

Real applications of MST for reinforced concrete and steel structural health monitoring remain highly promising, but undeveloped.

The aim of this project is to develop an MST system for passively monitoring the structural health of reinforced and steel concrete assets.

Approximately 125 tonnes of separated Pu is in long term storage at Sellafield

cumstances, gas generation may occur with consequent storage package pres-

surisation. In practice, this is rarely seen and empirically derived criteria are used to account for the release of known gases into the package and so ensure safe storage conditions. The purpose of this proposed PhD project is to contribute to a fundamental understanding of the factors influencing the empirical

as calcined PuO2 powder in nested, sealed steel storage cans. Under certain cir-



To be recruited PhD, University of Strathclyde

The Recombination of Hydrogen and Oxygen on Metal Oxide Surfaces



criteria.

To be recruited, PhD, Lancaster University

> Advanced characterisation of waste pipe flows with polymeric behavioural modifiers.



To be recruited, PhD, University of Leeds

Waste suspension flows are encountered across the nuclear sector, and their characterisation is of great importance to the safe transport of radioactive material. A waste treatment program that has received high priority in recent years, is the retrieval of legacy waste sludge from historical ponds to safe interim storage facilities. Suspension transfer via pipeline has encountered several problems resulting from a lack of relevant design data. As such, operations are often run with extreme caution and not necessarily at their optimum, which may cause further downstream problems. For example, to mitigate the potential for radioactive particles to block pipes, high flowrates are employed, leading to shear breakdown of aggregates that reduces waste consolidation rates downstream in the interim stores. This project seeks to understand these issues and overcome pipeline transportation problems in two ways – the development of an online acoustic backscatter technique for remote characterisation of particle size and concentration online, and the use of polymer additives to modify slurry characteristics enabling safe and efficient slurry transport.

Nanotechnology for effluent treatment and radionuclide assay

To be recruited PDRA Imperial College This project will build on the work done in the Distinctive consortium, where it was shown that phosphate functionalised paramagnetic iron oxide particles showed a surprisingly large capacity and selectivity for uranium sorption.

A first set of research objectives is to clarify further why what appears to be a multi-layer structure has such a large capacity.

A second objective is to widen the same approach to other radionuclides of interest. A third objective is to develop particles that can act in acidic environments.