Book of abstracts

Day of the PhDs

September 28, 2017

SCK•CEN
Boeretang 200
BE-2400 MOL
Belgium
http://www.sckcen.be

Organising committee

Dr Michèle Coeck (Head of the SCK•CEN Academy for Nuclear Science and Technology)

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Programme

Oral presentations

Morning session – Part I, chaired by the following PhD students

- Chao Yin (SMA)
- Oksana Klok (SMA)

08:30-09:00	Registration and welcome coffee	
09:00-09:15	Welcome & introduction	Michèle Coeck, Head SCK•CEN Academy for Nuclear Science and Technology Prof. Thomas Pardoen, President Scientific Council SCK•CEN
09:15-09:35	Finite element analysis of stress heterogeneity in tungsten polycrystal under ITER-relevant cyclic heat load	**Aleksandr Zinovev** SCK•CEN mentors: Dmitry Terentyev & Lorenzo Malerba University promoter: Laurent Dellanay, UCL Start date: October 1st, 2015
09:35-09:55	Updates and construction of the full SoLid detector	**Celine Moortgat** SCK•CEN mentors: Edgar Koonen & Lucia Popescu University promoter: Dirk Rykbosch, UGENT Start date: October 1st, 2014
09:55-10:15	Surface microstructure and retention after high flux He-D plasma exposures in recrystallized and heavily deformed tungsten	**Anastasia Bakaeva** SCK•CEN mentors: Dmitry Terentyev & Lorenzo Malerba University promoter: Jean-Marie Noterdaeme, UGENT Start date: November 15, 2014
10:15-11:00	Break + poster presentations	

Morning session – Part II, chaired by the following PhD students

- Martin Ashford (PTR)
- Kristof Gladinez (CCP)

11:00-11:20	Public opinion and nuclear energy: the role of national context	**Edwin Latré** SCK•CEN mentor: Tanja Perko University promoter: Peter Thijssen, UAntwerpen Start date: October 1st, 2014
11:20-11:40	Study of low Prandtl number heat transfer in the E-SCAPE liquid metal pool facility	**Edoardo Cascioli** SCK•CEN mentors: Katrien Van Tichelen & Steven Keijers University promoter: Sasa Kenjeres, TUDelft Start date: October 1st, 2015
11:40-12:00	Development and validation of a multi-scale simulation method for high-fidelity thermal-hydraulic analyses	**Antonio Toti** SCK•CEN mentors: Francesco Belloni & Gert Van den Eynde University promoter: Jan Vierendeels, UGENT Start date: November 1st, 2014
12:00-12:20	Development of carbide materials for radioactive ion beam production at high-power ISOL facilities	**Matteo Griseri** SCK•CEN mentors: Lucia Popescu & Konstantza Lambrinou University promoter: Jef Vleugels, KU Leuven Start date: October 15, 2016
12:20-13:30	Sandwich lunch + poster presentations	

Afternoon session – Part I, chaired by the following PhD students

- Emma Coninx (RDB)
- Pasquale Lombardo (RDA)

13:30-13:50	Atmospheric transport modelling in support of the Comprehensive Nuclear Test-Ban-Treaty	**Pieter De Meutter** SCK•CEN mentor: Johan Camps RMI mentor: Andy Delcloo University promoter: Piet Termonia, UGENT Start date: January 1st, 2015
13:50-14:10	How do different radiation qualities affect the Hedgehog signaling pathway in cancer cells?	**Katrien Konings** SCK•CEN mentor: Marjan Moreels University promoter: Karin Haustermans, KU Leuven Start date: October 1st, 2014
14:10-14:30	High-throughput monitoring of BR2 aquatic microbial communities through combined flow cytometry and metagenomics	**Ruben Props** SCK•CEN mentors: Pieter Monsieurs & Natalie Leys University promoter: Nico Boon, UGENT Start date: October 13, 2014
14:30-15:00	Break + poster presentations	

Afternoon session – Part II, chaired by the following PhD students

- Noami Daems (RDB)
- Niels Belmans (RDB)

15:00-15:20	A simulation platform for virtual clinical trials in chest X-ray imaging	**Sunay Rodriguez Perez** SCK•CEN mentors: Lara Struelens & Filip Vanhavere University promoters: Hilde Bosmans & Nicholas Marshall, KU Leuven Start date: December 15, 2014
15:20-15:40	2 years of space and hadron therapy dosimetry with luminescent detectors	**Alessio Parisi** SCK•CEN mentors: Olivier Van Hoey & Filip Vanhavere University promoter: Patrice Mégret, UMons Start date: October 1st, 2015
15:40-16:00	Personal dosimetry of workers without a physical dosimeter: an innovative application using computational methods	**Mahmoud Abdelrahman** SCK•CEN mentors: Filip Vanhavere & Lara Struelens University promoters: Christophe Phillips & Alain Seret, Ulg Start date: August 16, 2016
16:00-16:05	Closure	Prof. em. Michel Giot, Honorary President of the Scientific Council SCK•CEN
16:05	Drink	

Poster presentations

Within the Institute Advanced Nuclear Systems (ANS)

Target design-optimisation for the 100 MeV proton target facility	**Martin Ashford** SCK•CEN mentor: Lucia Popescu University promoter: Hamid Aït Abderrahim, UCL Start date: January 1st, 2017
Mass transport of oxygen and corrosion products in LBE cooled systems	**Kristof Gladinez** SCK•CEN mentors: Kris Rosseel & Jun Lim University promoter: Geraldine Heynderickx, UGENT Start date: October 1st, 2015

Within the Institute Environment, Health and Safety (EHS)

Modelling of drying shrinkage in concrete; a multiscale pore-network approach	Saeid Babaei SCK•CEN mentors: Lou Areias & Suresh Seetharam University promoters: Gunther Steenackers & Bart Craeye, UAntwerpen Start date: January 15, 2017
Age-related biological effects of dental cone-beam CT exposure	Niels Belmans SCK•CEN mentors: Marjan Moreels & Sarah Baatout University promoters: Ivo Lambrichts, UHasselt & Stéphane Lucas, UNamur Start date: October 1st, 2015
A hybrid Krylov-balanced Truncation model reduction technique	Gunther Bijloos SCK•CEN mentor: Johan Camps University promoter: Johan Meyers, KU Leuven Start date: October 1st, 2016
137Cs sorption on glauconite sands of the Neogene	Yaana Bruneel SCK•CEN mentors: Liesbeth Van Laer & Norbert Maes NIRAS mentor: Stéphane Brassines University promoter: Erik Smolders, KU Leuven Start date: October 1st, 2016
Polydispersity and polyfunctionality of Boom clay dissolved organic matter	Yulia Buchatskaya SCK•CEN mentors: Sonia Salah & Delphine Durce University promoter: Michel Devillers, UCL Start date: October 1st, 2016
The hippocampus: a target for premature aging after early life-irradiation	Emma Coninx SCK•CEN mentors: Mieke Verslegers & Roel Quintens University promoter: Lieve Moons, KU Leuven Start date: October 1st, 2016

Foliar uptake of Cs137 by spinach at different growth stages: experimental setup and preliminary data on interception fractions	Antonella Cristina SCK•CEN mentor: Lieve Sweeck University promoter: Roeland Samson, UAntwerpen Start date: November 1st, 2016
Cytotoxicity assessment of gold nanoparticles on non-cancerous cell lines	Noami Daems SCK•CEN mentors: An Aerts & Cagno Simone University promoters: Stéphane Lucas & Carine Michiels, UNamur Start date: October 17, 2016
Towards Bismuth-213-labeled nanobodies, a new treatment approach in Targeted Alpha Therapy	Yana Dekempeneer SCK•CEN mentors: Mireille Gysemans & Dominic Maertens University promoters: Vicky Caveliers & Matthias D'Huyvetter, VUB Start date: October 1st, 2016
Differences in radio sensitivity to gamma radiation between rice and Arabidopsis	Jackline Kariuki Mwihaki SCK•CEN mentors: Nele Horemans & Eline Saenen University promoter: Ann Cuypers, UHasselt Start date: October 1st, 2015
Direct sampling VS our new multiphase-multiresolution simulated annealing approach: which porous media reconstruction looks best?	Laurent Lemmens SCK•CEN mentors: Eric Laloy & Mieke Decraen University promoters: Marijke Huysmans & Rudy Swennen, KU Leuven Start date: October 1st, 2016
Uranium isotopic composition determination using CdZnTe and LaBr3 detectors	Iaroslav Meleshenkovskii SCK•CEN mentors: Alessandro Borella & Michel Bruggeman University promoters: Nicolas Pauly & Pierre-Etienne Labeau, ULB Start date: September 1st, 2015
Internal gelation process for the production of simulated transmutation fuel particles	Christian Schreinemachers SCK•CEN mentors: Cagno Simone & Marc Verwerft University promoter: Koen Binnemans, KU Leuven Start date: October 1st, 2016
On the capillarity and micro-structure of hardened cement paste: a multidisciplinary study	Timo Seemann SCK•CEN mentors: Norbert Maes & Diederik Jacques NIRAS mentors: Séverine Levasseur & Seif Ben Hadj Hassine University promoters: Veerle Cnudde, UGENT & Amir Raoof, UUtrecht Start date: October 17, 2016
Characterization of carbonation-induced changes in roughness of crack surfaces in hardened cement pastes	Anna Varzina SCK•CEN mentors: Janez Perko & Norbert Maes University promoter: Özlem Cizer, KU Leuven Start date: October 6, 2016
On-line coupling of HPLC with ICP-MS for elemental and isotopic analysis of spent nuclear fuel	Nancy Wanna SCK•CEN mentors: Karen Van Hoecke & Mirela Vasile University promoter: Frank Vanhaecke, UGENT Start date: January 15, 2017

Within the Institute Nuclear Materials Science (NMS)

Chemical compatibility of select MAX phases with static Lead-Bismuth Eutectic (LBE)	Bensu Tunca SCK•CEN mentors: Konstantza Lambrinou & Rémi Delville University promoters: Jef Vleugels, KU Leuven & Joke Hadermann, UAntwerpen Start date: October 1st, 2015
Defect clustering and long-range ordering in UO2+x and higher valence phases	Emre Caglak SCK•CEN mentor: Kevin Govers University promoter: Alain Dubus, ULB Start date: November 16, 2016
Characterization of 24% cold worked DIN 1.4970 steel after ageing	Niels Cautaerts SCK•CEN mentors: Rémi Delville & Erich Stergar University promoter: Dominique Schryvers, UAntwerpen Start date: October 1st, 2015
Calorimetric studies of the U-Mn and U-Al binary systems	Andrew Cea SCK•CEN mentors: Sven Van den Berghe & Ann Leenaers University promoter: Thomas Pardoen, UCL Start date: October 1st, 2016
Developing of the advanced FOCS system for ITER and WEST	Anton Miazin SCK•CEN mentors: Andrei Goussarov & Willem Leysen University promoters: Marc Wuilpart & Patrice Mégret, UMons Start date: November 15, 2016
Pore pressure estimation in irradiated UMo	Daniele Salvato SCK•CEN mentors: Sven Van den Berghe & Ann Leenaers University promoters: Christophe Detavernier, UGENT Start date: November 1st, 2016
Mechanical properties and fracture surface of baseline and novel tungsten for fusion application	Chao Yin SCK•CEN mentors: Dmitry Terentyev & Andrei Goussarov University promoters: Thomas Pardoen, UCL & Roumen Petrov, UGENT Start date: January 15, 2017

Oral presentations

Finite element analysis of stress heterogeneity in tungsten polycrystal under ITER-relevant cyclic heat load

Aleksandr Zinovev
Institute Nuclear Materials Science
Expert Group Structural Materials

SCK•CEN mentors: Dmitry Terentyev & Lorenzo Malerba
University promoter: Laurent Delannay (UCL)
Start date as PhD: October 1st, 2015

Abstract

Nowadays there is a big scientific challenge: designing and construction of a fusion reactor which will have considerable benefits over fission reactors. The largest fusion device ITER is currently under construction in France, while its successor DEMO is in the conceptual design stage. Tungsten is selected as plasma-facing material for ITER and DEMO due to envisaged severe operational conditions, namely neutron irradiation and cyclic heat loads. The latter will lead to thermal fatigue and initiation of surface cracks, while their propagation is detrimental for the structural integrity of armour monoblocks, being a safety concern.

Published papers devoted to finite element analysis (FEA) of crack initiation at the surface of tungsten subjected to cyclic heat loads have considered homogenous and isotropic material model only. But as long as cracks primarily initiate at the grain boundaries and triple junctions, as well as due to anisotropic nature of deformation of individual grains, the knowledge of stress and strain heterogeneity in grains is essential for accurate prediction of cracking.
Crystal plasticity (CP) is required to account for the interaction of every grain with its neighbours during plastic deformation. Coupled with FEA, CP is used to predict the stress and strain heterogeneity within each grain, and thus, identify positions of possible crack initiation. Potential paths for intergranular crack are represented by cohesive zone elements, which connect the adjacent volume finite elements, and are characterized by the traction-separation law, which controls the crack opening.

First, a strain hardening law, based on a modified Kocks-Mecking model, was developed to reproduce uniaxial tensile tests of tungsten with the help of FEA. The obtained law of mechanical behaviour was then used in the simulations of a tungsten sample subjected to ITER-relevant cyclic heat loads to calculate thermally-induced strain and stress. Strain state at selected points of interest of the macroscopic sample was applied at the microscopic level to an aggregate of grains, where CP was used on a FE mesh. Cohesive elements with high stiffness and unattainable strength were placed along grain boundaries in order to probe the stress along the potential crack paths.

Updates and construction of the full SoLid detector

Celine Moortgat
Institute Nuclear Material Sciences
Expert Group BR2

SCK•CEN mentors: Edgar Koonen & Lucia Popescu
University promoter: Dirk Rykbosch (UGENT)
Start date as PhD: October 1st, 2014

Abstract

Neutrinos have been the subject of many particle physics experiments and over a few decades a clear picture of 3 oscillating neutrino flavours has been built. Although the experimental confirmation of this theory received the Nobel Prize in Physics in 2015, some experimental data sets appear incompatible with this framework. Clues from accelerator set-ups, source calibration of solar neutrino experiments and re-evaluation of short baseline reactor experiments are possibly pointing to the existence of new physics. These anomalies could be explained by introducing a 'sterile' neutrino, which does not interact via the weak interaction and can therefore not be detected directly.

New experiments are needed to confirm or set limits on the existence of this particle beyond the Standard Model of physics. The SoLid experiment will study this hypothesis by performing a short-baseline experiment at the BR2 reactor in Mol. A new detector technology together with a unique location such as the BR2 reactor will provide a huge advantage over our competitors.

The technology that makes SoLid stand out from other sterile searches is the use of a composite solid scintillator. The detector will be constructed out of 12800 PVT scintillator cubes, with a volume of 5 cm^3 each, that are each equipped with 2 ^{6}Li:ZnS sheets and wrapped individually in Tyvek so as to optically isolate them from the other cubes in the detector. The large-scale use of this technology has been tested by building and taking data with a prototype module during the first 2 years of this thesis. Even though the prototype data validates the SoLid technology, it also shows where to make upgrades to the full SoLid detector. This detector, called Phase 1, is under construction at the moment and it is expected to start taking data during the last BR2 reactor run of 2017. Phase 1 will be able to perform a sensitive oscillation search after a few years of data taking.

This presentation will give an overview of the analyses performed on the prototype data set, the upgrades applied to the Phase I detector and construction of the sensitive volume of the detector at the University of Ghent. Also an outlook will be given on the cosmogenic background study, which will be performed during the last year of this thesis and is needed to better distinguish the antineutrino signal that SoLid is looking for.

Surface microstructure and retention after high flux He-D plasma exposures in recrystallized and heavily deformed tungsten

Anastasia Bakaeva
Institute Nuclear Materials Science
Expert Group Structural Materials

SCK•CEN mentors: Dmitry Terentyev & Lorenzo Malerba
University promoter: Jean-Marie Noterdaeme (UGENT)
Start date as PhD: November 15, 2014

Abstract

Due to its advantageous thermal properties, tungsten will be used as the plasma-facing material for the ITER divertor. Bombardment of tungsten with low-energy high flux plasma ions, such as deuterium, tritium and helium, leads to surface modifications (e.g. blistering, swelling, etc.) which depend on irradiation conditions. A synergy of He-H interaction results in the formation of sub-surface bubbles and suppresses the diffusion of H isotopes deeper into the bulk. Hence, understanding of the mutual interaction of He with H-isotopes and subsequent evolution of the microstructure is an important subject to study.

In this work, we investigate the retention and microstructural evolution under high flux (i.e. 10^{24} ions/m^2/s) deuterium-helium plasma exposure while varying the content of He in a wide range. A particular goal was to study the influence of He seeding in D plasma on the trapping and release in reference and plastically-deformed ITER specification tungsten grades. Thermal Desorption Spectroscopy (TDS) measurements were performed to reveal the main release stages and the role of plastic deformation on the retention under pure He and He-seeded exposures. By comparison of the results obtained in the mixed exposures with previous data obtained for pure D exposures, we aim to single out the impact of He and the role played by He-seeding in the mixed plasma beam. Therefore, high resolution TDS was used to clarify the features of simultaneous release in the exposures made using the reference samples, while a standard quadruple mass spectrometer was used to study the impact of plastic deformation.

In addition to TDS investigations, Transmission Electron Microscopy (TEM) examination of the sub-surface layer was made to reveal the impact of the plasma exposure on the microstructure and nanoindentation was applied to reveal the modification of surface hardness. Plasma shots were found to result in the localized plastic deformation, seen as dense dislocation lines, and in the formation of nano-metric cavities of high density.

Public opinion and nuclear energy: the role of national context

Edwin Latré
Institute Environment, Health and Safety
Expert Group Society and Policy Support, Nuclear Science and Technology Studies Unit

SCK•CEN mentor: Tanja Perko
University promoter: Peter Thijssen (UAntwerpen)
Start date as PhD: October 1st, 2014

Abstract

In many countries, there is an ongoing debate about the role of nuclear energy in the energy mix. This debate is fuelled by the need to guarantee energy security, while also tackling the problem of climate change (EC, 2010). In these debates, national actors – such as the media and political parties – play an important role (Müller & Thurner, 2017). This PhD research focuses on how these national actors affect public opinion formation about a complex and technological issue such as nuclear energy. To study the relationship between national actors and public opinion we first focus on periods of increased political attention for nuclear energy policy, for example, after the Fukushima nuclear accident. Different research designs are used that enable us to look both at the aggregate and at the individual level; A large-N comparative design of 41 countries, a small-N comparative design and a single case study (i.e. Belgium with the SCK•CEN barometer data).

Our first results (study 1) indicate that previous research has somehow misunderstood the moderating role of national context on opinion change after the Fukushima accident. An analysis of a survey conducted shortly after the accident with more than 23,000 respondents from 41 countries revealed that the decrease in support for nuclear energy was stronger in countries closer to Fukushima. In addition, support for nuclear energy decreased more in countries where new nuclear reactors were under construction. However, the country's nuclear energy production status and press freedom did not determine opinion change after the Fukushima accident. The non-effect of freedom of the press on opinion change contradicts the role of media after a focusing event as described in the literature. Overall results demonstrate a limited effect of national context on opinion change following a focusing event. However, this does not mean that national context is not an important determinant for the initial level of support for nuclear energy.

In-depth research on opinion formation and politicization within Belgium showed that knowledge of the parties' positions on the nuclear energy is low. However, people who intend to vote for one of the parties more active in the politicization of nuclear energy have a more consistent belief system on the issue and use partisan cues when forming an opinion about nuclear energy (study 2). In sum, via the mechanism of cue taking, political elites can polarize public opinion on nuclear energy. This is an important addition to the dominant psychometric model that is used to explain public opinion vis à vis nuclear energy. Furthermore, in study 3 we will show how that the influence of the political context on public support for nuclear energy is to a large extent mediated by national media. Notably, we see important differences in the level of support for the casualties of the Fukushima accident between Flemish and Walloon respondents which seem to be related to differential media framing.

Study of low Prandtl number heat transfer in the E-SCAPE liquid metal pool facility

Edoardo Cascioli
Institute Advanced Nuclear Systems
Expert Group Nuclear Systems Research, LBE Components and Experiments Unit

SCK•CEN mentors: Katrien Van Tichelen & Steven Keijers
University promoter: Sasa Kenjeres (TUDelft)
Start date as PhD: October 1st, 2015

Abstract

Liquid metal-cooled fast reactors can contribute to the future of nuclear energy production thanks to the possibility of using more efficiently the natural resources and reducing the amount and lifetime of nuclear waste. At SCK•CEN, the Multi-purpose hYbrid Research Reactor for High-tech Applications (MYRRHA) is being designed to be a pool-type fast reactor prototype cooled by Lead-Bismuth Eutetic.

Thermal hydraulics is recognized as a key aspect in the design phases and safety analyses. Three-dimensional flows of liquid metal in natural and forced convection regimes need to be carefully investigated, modelled and tested for pool-type systems.

In the solution of the Reynolds Averaged Navier-Stokes (RANS) equations for fluid flow, current engineering computational fluid dynamics tools apply statistical turbulence closure, adopting the concept of a turbulent Prandtl number based on the Reynolds analogy. The main assumption is here that the turbulent heat flux in the time-averaged energy equation can be modelled analogous to the Reynolds stresses in the time-averaged momentum equation. This hypothesis is valid mainly for forced convection flows and fluids with a molecular Prandtl number of the order of unity. Because of their high thermal conductivity, liquid metals are characterized by significantly lower values of the molecular Prandtl number.
Hence, the goal of the PhD is the development of an innovative RANS turbulent heat transfer model for low Prandtl number fluids for industrial use with particular reference to fast pool-type reactors cooled by liquid metals.

Parametric studies have been performed for wall and free shear flows setting different molecular and turbulent Prandtl numbers in order to estimate and physically understand the sensitivity of the standard RANS approach to these properties of the fluid and flow respectively.
Large-eddy simulations are also being performed for the same fundamental test cases. This numerical database will be complemented with experimental data from the operation of a wind tunnel with a mixture of low Prandtl number noble gases under construction at The von Karman Institute for Fluid Dynamics.

These achievements will represent the basis to select and improve the current low Prandtl number heat transfer correlations and models, suitable only for few specific flow regimes. The developed turbulent heat transfer model will be finally tested and optimized with experimental data from the European SCAled Pool Experiment (E-SCAPE) facility, a thermal-hydraulic 1/6-scale model of the MYRRHA reactor built and operated by SCK•CEN.

Development and validation of a multi-scale simulation method for high-fidelity thermal-hydraulic analyses

Antonio Toti
Institute Advanced Nuclear Systems
Expert Group Nuclear Systems Physics

SCK•CEN mentors: Francesco Belloni & Gert Van den Eynde
University promoter: Jan Vierendeels (UGENT)
Start date as PhD: November 1st, 2014

Abstract

The safety assessments of nuclear installations, carried out to support the design, licensing and operation, require sophisticated computational tools able to accurately predict the response of the system to operational and accidental transients, and the potential consequences on safety related parameters. Pool-type liquid metal-cooled reactors, such as the MYRRHA irradiation facility, are challenging from this point of view due to the complex multi-dimensional nature of the coolant flow in the primary system, and the presence of local thermal-hydraulic phenomena that can influence the system dynamic characteristics.

In order to improve the currently available modelling and simulation capabilities, a multi-scale computational method based on the use of coupled system thermal-hydraulic (STH) and CFD codes is investigated in this PhD research activity. The developed method is based on domain decomposition, and novel numerical algorithms have been implemented and successfully tested. Within the verification and validation (V&V) programme outlined for the numerical tool, a coupled model has been developed for the analysis of the scaled facility E-SCAPE, built at SCK•CEN. The computational method is applied on the pre-test analysis of loss of flow (LOF) transients, involving the complex transition from forced to natural circulation flow in the primary system. The results confirmed that the transient behaviour of a pool-type system is characterized by complex flow and temperature fields, difficult to predict by the industry-standard STH codes.
The experimental tests will be used for the validation of the tool, in the view of its use to support the design and licensing of MYRRHA. In parallel, coupled analyses are being performed on the MYRRHA reactor and compared against stand-alone STH results.

Development of carbide materials for radioactive ion beam production at high-power ISOL facilities

Matteo Griseri
Institute Advanced Nuclear Systems
Expert Group Accelerator Project, Proton Target Research Unit

SCK•CEN mentors: Lucia Popescu & Konstantza Lambrinou
University promoter: Jef Vleugels (KU Leuven)
Start date as PhD: October 15, 2016

Abstract

ISOL@MYRRHA is a project of SCK•CEN dedicated to the construction of an ISOL facility exploiting the 600 MeV accelerated proton beam that is foreseen for the ADS reactor MYRRHA. In an ISOL facility, accelerated protons irradiate a target material from where reaction products are extracted, ionized, selected according to the Z and A number and utilized in the form of isotopically pure RIBs (Radioactive Ion Beams). Applications of RIBs range from research in fundamental physics to radio-biology. Of specific interest is ^{149}Tb for radio-pharmaceutical research. The choice of the target material begins with the selection of atomic species with a high production cross-section for the desired isotopes. Tantalum, hafnium and gadolinium were selected due to their high cross-section for production of lanthanides through spallation at 600 MeV (Ta and Hf) and at 100MeV (Gd). Evaporation of the reaction products must be ensured by a high surface to volume ratio (S/V), obtained for instance by interconnected porosity in the target material. ISOL@MYRRHA proposes to operate on a single target for up to 4 weeks of irradiation with a high intensity proton beam (~100 µA). Temperatures in the target will reach around ~2000°C and boost the in-grain diffusion of reaction products. These harsh operating conditions ultimately impose constraints on the melting point and thermal conductivity of the material, as well as its geometry. Refractory carbide ceramics based on Ta, Hf and Gd are considered promising candidate target materials, hence the first phase of this PhD project focused entirely on the synthesis, characterization and microstructural fine tuning of these materials. The FLUKA code will simulate the in-target production rate of isotopes and heat deposition, allowing geometry optimization. At last, the selected target material will be tested at existing facilities such as ISOLDE (CERN) and ISAC (TRIUMF, Canada). Porous TaC was obtained via dealumination of Ta_4AlC_3 MAX phase. These ternary ceramics are composed of a transition metal M (Ta in this case), a metalloid A (Al) and C or N, arranged in a hexagonal lattice. Ta_4AlC_3 specimens were produced by reactive sintering of elemental size-tailored powders. A reproducible process for the synthesis of phase-pure Ta_4AlC_3 MAX phase was developed. Porous $TaC_{0.75+x}$ is obtained when the Al is removed from the Ta_4AlC_3 by heat treatment. This process will be further explored in order to fully control the pore formation and microstructure. Spark Plasma Sintering (SPS) of commercial TaC powder was performed as an alternative route to obtain micro-porous materials with 40% open porosity. Thermal conductivity measurements at high temperature will be performed to understand how the porosity influences the heat transfer in the material. The possibility to include Gd as a dopant in ZrC was explored by carbo-thermal reduction of Gd_2O_3-coated zirconia. More work is needed to understand how to control the phase formation and densification. The final goal is to select a material that accommodates the requirements and that can be synthesized in a simple and reproducible process.

Atmospheric transport modelling in support of the Comprehensive Nuclear Test-Ban-Treaty

Pieter De Meutter
Institute Environment, Health and Safety
Expert Group Society and Policy Support, Crisis Management and Decision Support Unit

SCK•CEN mentor: Johan Camps
RMI mentor: Andy Delcloo
University promoter: Piet Termonia (UGENT)
Start date as PhD: January 1st, 2015

Abstract

The Comprehensive Nuclear Test-Ban-Treaty aims to ban nuclear explosions globally. An International Monitoring System is being setup that will be used to verify compliance with the Treaty. It consists of hydro acoustic, infrasound and seismic wave observations, and the detection of radionuclides in the atmosphere. The latter is of particular importance since it allows to discriminate conventional explosions from nuclear explosions. Radioactive noble gases (^{131m}Xe, ^{133}Xe, ^{133m}Xe and ^{135}Xe) and radioactive particulates are being monitored. If one or multiple radionuclides are detected in the atmosphere, atmospheric transport modelling can be used to determine the origin. This is a challenging task due to several reasons, ranging from computation cost to the chaotic nature of the atmosphere and the existence of a background of radioactive xenon coming from civil sources, mainly medical isotope production facilities and nuclear power plants.

Here we give an overview of the work on atmospheric transport modelling that has been done in support of the Comprehensive Nuclear Test-Ban-Treaty. We will present an analysis of suspicious ^{133}Xe detections after the 4th announced nuclear test conducted by the Democratic People's Republic of Korea in January 2016, with emphasis on the uncertainty quantification of atmospheric transport modelling. Furthermore, work on the intrinsic temporal resolution of current operational atmospheric transport models will be presented, which allows giving recommendations on the temporal resolution of emission data of civil sources. Possibly work dealing with the recent announced nuclear test by the Democratic People's Republic of Korea on the 3rd of September 2017 will be discussed.

How do different radiation qualities affect the Hedgehog signaling pathway in cancer cells?

Katrien Konings
Institute Environment, Health and Safety
Expert Group Interdisciplinary Biosciences, Radiobiology Unit

SCK•CEN mentor: Marjan Moreels
University promoter: Karin Haustermans (KU Leuven)
Start date as PhD: October 1st, 2014

Abstract

In recent years an increase is observed in the use of particle therapy (protons, carbon ions) for the treatment of cancer patients. This is in part because of the advantages of particles compared to X-rays, which include an increased biological effectiveness and improved sparing of healthy tissues. Metastasis is still an important cause of mortality in cancer patients and evidence shows that conventional radiotherapy could actually increase the formation of metastasizing cells. An important pathway implicated in the process of metastasis is the Hedgehog (Hh) signaling pathway. Recent studies demonstrated that activation of this pathway in response to photon exposure can lead to radioresistance and increased invasive and migratory capability of cancer cells. Currently, the impact of particle radiation on the Hh signalling pathway is unknown.
The effect of different radiation qualities (photons, protons and carbon ions) on the Hh signaling pathway was investigated in prostate cancer cells (PC3), paediatric medulloblastoma cells (DAOY) and breast cancer cells (MCF-7). More specifically we were interested in the effect of irradiation on radiosensitivity and potential modulation by GANT61, the gene expression of the Hh pathway and the migratory potential of the cancer cells. Experiments with X-rays were performed at SCK•CEN (Mol, Belgium) whereas experiments with protons were performed at the iThemba facility in South-Africa and with carbon ions at the Grand Accélérateur National d'Ions Lourds (GANIL) (Caen, France).

Carbon ion irradiation was more effective in decreasing cell survival compared to X-rays (RBE_{10} = 2.0 for PC3 cells; RBE_{10} = 2.1 for DAOY cells; and RBE_{10} = 2.2 for MCF-7 cells). The Hedgehog inhibitor GANT61 did not have a radiosensitizing effect in PC3 cells in combination with any of the radiation qualities. However, a radiosensitizing effect of GANT61 could be observed in the DAOY cells after proton and carbon ion irradiation and in MCF-7 cells after carbon ion irradiation. Gene expression analysis showed that the response of the Hedgehog pathway genes was dependent on the irradiation type, cell type and time after irradiation. In general, carbon ion irradiation induced more pronounced changes in gene expression compared to X-ray irradiated samples. Finally, the migratory capacity of DAOY cells decreased in a radiation dose dependent manner, with a more pronounced decrease of migration after proton and carbon ion irradiation compared to X-ray irradiation. This decrease was also observed for PC3 cells but only after carbon ion irradiation.
In conclusion, carbon ion irradiation was more potent, compared to X-rays, in inducing cell killing, affecting the expression of the Hh pathway genes and decreasing migration. These results highlight again the biological differences between X-ray and particle irradiation. The radiosensitizing effect of GANT61 in combination with particle therapy can be of interest for the clinic because lower doses of irradiation are need for treatment and thus the surrounding normal tissues will also receive less dose. Future experiments with Hh inhibitors will address whether modulation of the Hh pathway will differentially affect migration capacities of cancer cells after exposure to different radiation qualities.

High-throughput monitoring of BR2 aquatic microbial communities through combined flow cytometry and metagenomics

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Abstract

Microbial diversity has been shown to be an important community property for preserving community functionality and preventing pathogen invasion. Despite the availability of high-throughput sequencing technologies, there exists a need for assessing the diversity on a rapid, inexpensive and database-independent platform with limited computational effort. Here, we demonstrate that sensitive single-cell measurements of phenotypic attributes, obtained via flow cytometry, can provide fast first-line assessments of microbial diversity dynamics, without demanding extensive sample preparation and downstream data processing. By calculating established diversity metrics from whole-community cytometric data, we constructed an alternative interpretation of microbial diversity that incorporates distinct phenotypic traits underlying cell-to-cell heterogeneity (i.e., morphology and nucleic acid content). Using 16S rRNA gene amplicon sequencing as a benchmark, we evaluated the extent to which our developed biodiversity indices capture shifts in the taxonomic composition of planktonic microbial communities spanning a large diversity gradient. For this purpose we sampled the secondary cooling water ecosystem of the BR2 nuclear reactor throughout two 30-day reactor cycles, and a productivity gradient within Lake Michigan (US), one of the largest freshwater ecosystems in the world. Our newly developed approach correlated strongly with the benchmark diversity and was proficient in detecting shifts in community composition. As such, we showed that our advanced analysis of flow cytometry data represents a novel and powerful resource, capable of detecting microbial community shifts. Our computational method is publicly available as an R software package (https://github.com/rprops/Phenoflow_package) and can be directly applied in baseline monitoring of engineered aquatic systems.

In particular for the BR2 secondary cooling water system, the microbial community dynamics were dictated by three bacterial taxa (>80 % of community). Detailed metagenomic analysis resulted in the complete recovery of these three bacterial genomes, without significant contamination or fragmentation. It could be shown that these genomes were similar in size (3.4 - 3.9 Mbp) but varied greatly in %GC, an indication for differing selection pressure. The most abundant organism, a *Limnohabitans* sp., was the only organism that carried the (near-)complete chemotaxis and motility pathways. It also has no known close relatives in public databases, and has a high codon bias in coding DNA sequences, suggesting that this organism may have a highly efficient protein-production apparatus. Overall these results indicate that the microbial community of an ultra-oligotrophic environment such as the BR2 cooling water system selects for a low-diversity microbial community containing organisms with highly differing genomic and functional features. Currently, metabolic modelling of this community is being performed which will reveal the exact metabolic dependencies between these organisms.

A simulation platform for virtual clinical trials in chest X-ray imaging

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Abstract

The aim of optimization of chest radiography is to ensure that image quality remains adequate for the clinical tasks undertaken while patient exposure is kept as low as possible. Establishing good image quality is a complex subject as this is strongly linked to the clinical task. Additionally, the evaluation of a large number of system parameters is necessary. While clinical trials offer the gold standard in terms of tasks, realism and observer performance, aspects such as cost, duration and the inevitable patient to patient variation are limitations. In contrast, virtual clinical trials (VCT), in which computer simulations are used to model the image acquisition, processing and reading process, constitute a more practical alternative. Anthropomorphic computational phantoms can be used as anatomical models of real patients.

This work describes the creation of a simulation framework for VCT of chest X-rays. A methodology for simulating the imaging chain was developed and validated in terms of image quality and dose using simple homogeneous structures. Radiographic images were generated via Monte Carlo modelling in conjunction with ray tracing methods. Measured detector imaging characteristics, given by presampling modulation transfer function (MTF) and the noise power spectrum (NPS) were used to apply realistic degrees of sharpness and noise to the simulated images. This simulation framework has now been extended to include a focused anti-scatter grid. A set of chest anthropomorphic phantoms were created and diverse clinical tasks were added: lung nodules, catheter and rib fractures. Future evaluation will include an observer study, where the generated image dataset will be evaluated by radiologists.

2 years of space and hadron therapy dosimetry with luminescent detectors

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Abstract

This talk describes some of the most relevant findings and results achieved during the first two years of my PhD research at the Belgian Nuclear Research Centre SCK•CEN. The goal of this work is to improve the dosimetry in complex radiation environments such as space and hadron therapy beams by combining different types of luminescent detectors with Monte Carlo radiation transport simulations. The PhD work can be subdivided in four main categories: detector characterization, radiation transport simulations, measurements in space and measurements in hadron therapy beams. Each part will be briefly discussed during the talk and a short summary is given hereunder.

Characterization of detectors for space and hadron therapy applications
Thermoluminescent (TL) and optically stimulated luminescent (OSL) detectors have been exposed in heavy charged particle accelerators and at the LNK lab of SCK•CEN. The main results and the practical implications of the findings will be presented.

Monte Carlo radiation transport simulation and microdosimetric modeling
Simulations of the irradiation setup used for detector characterization are needed to better understand the response of the detectors. This will be shortly discussed during the talk together with the description of the development and benchmark of a new microdosimetric model able to predict the efficiency of luminescent detectors exposed to charged particles.

Measurement in space
I am currently involved in the DOSIS-3D dose mapping experiment aboard the Columbus module of the International Space Station for the preparation, reading and analysis of the SCK•CEN space detector packages. A general overview of the project and the last results will be given.

Measurements in hadron therapy beams
I have collaborated with the EURADOS work group 9: Mailed dosimetry auditing in Proton Therapy providing support for detector preparation, reading and analysis. Furthermore, I am part of a dosimetry-biology combined measurement campaign aiming to assess in-field and out-of-the-field radiation doses delivered during proton therapy treatments and their relative biological effectiveness. The aim and the experimental setup of the first measurements performed in the proton therapy beam of iThemba Labs (Cape Town, South Africa) will be described.

Personal dosimetry of workers without a physical dosimeter: an innovative application using computational methods

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Abstract

Personal dosimetry is used mainly to ascertain doses to workers who are occupationally exposed to ionizing radiation. For more than 50 years now, passive dosimeters are being used to assess the dose to workers. This dosimeter is designed to measure the operational quantity $H_p(10)$ as an estimate of the effective dose E which is a quantitative measure of the "radiation detriment" that cannot be measured directly. The results are mostly known only after some time with passive dosimeters, and wearing a dosimeter is often seen as a burden by some workers. Also the uncertainties with the present dosimeters (within a factor of 1.5 or 2 from the real value) are not negligible.

Recent developments are moving towards active personal dosimetry. This would improve the application of the ALARA principle. On the other hand, computational techniques are also evolving fast and very detailed computational voxel/NURBS phantoms that represent realistic human anatomy are now available. On these NURBS phantoms it is feasible to do Monte-Carlo simulations so that organ doses from any radiation field can be calculated. With increasing computational power, such calculations go faster and faster.

We are developing an innovative application based on real-time computational methods to determine occupational exposures. The idea of this PhD is to make an application in which, for a certain workplace field, doses to workers will be calculated instead of measured. For this the spatial radiation field, including energy and angular distribution, needs to be known and can be incurred from on-line dose measurements on several locations. The real movement of the persons is monitored using Time-of-Flight cameras, and transferred to the calculation tool. By this way, the non-measurable quantities either the effective dose or the organ doses that quantify the risk of ionizing radiation can be calculated and monitored.

During the first year of the PhD, we started with the exploration of the methodology. A tool to track a person in 3D coordinates using Microsoft® Kinect™ was developed and several dose calculations were performed using both deterministic and Monte-Carlo methods. A first series of experiments were performed. An anthropomorphic phantom was positioned on a moveable table in the horizontal room of the Laboratory for Nuclear Calibration (LNK). This table was moved to different distances from a Cs-137 source. The position of the phantom was monitored with the Kinect™ and the coordinates recorded. The dose to the phantom was calculated in different methods and compared: 1. using the reference values from the LNK 2. using VISIPLAN-3D 3. using MCNP simulations 4. using dosimeters. This experiment was repeated with different degrees of complexity of the movement of the phantom. Also the simulations were done with increasing detailed input, and increasing frequency. The results showed the validity of the methodology used in that test.

Next step will focus mainly on developing an algorithm to localize and inferring source strength from few dose measurement points. A second series of experiments are foreseen as well with increased level of complexity.

Poster presentations

Target design-optimisation for the 100 MeV proton target facility

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Abstract

Production of exotic Radioactive Ion Beams (RIBs) is a challenge, as these nuclei generally have very short half-lives, which makes off-line separation techniques (chemical, mass separation) less efficient, if not outright impossible (isotopes would decay before separation).

The Isotope Separation On-Line (ISOL) technique avoids these pitfalls by having both production and separation in one continuous process. The technique makes use of a light particle beam (here, protons) impinging onto a high-Z target material, inducing spallation, fragmentation and fission reactions, where the isotopes are produced. By heating the target material to a high temperature, these nuclei will be released from the bulk of the material through diffusion and effusion processes. They are then guided towards an ion source where they will be selectively ionised, and then extracted towards an on-line mass-separator.
The produced isotopes can then be used as they are, or post-accelerated if necessary.

The design of new targets is essential to optimising the production of these RIBs. Design is constrained by the necessity of maintaining target temperature within a narrow range (2000-2200 ºC), in order to ensure diffusion of the produced isotopes. A Monte-Carlo particle physics code and a finite-element thermo-dynamic solver were coupled to estimate production rates, heat deposition and temperature spread throughout the target system.
Several designs were tested, based on results from other facilities. Advantages and disadvantages were evaluated and will serve to guide the design of more optimal targets in the near future. Release (diffusion and effusion from the target material) and ionisation were not modelled at this time, as they are a lesser constraint for the longer-lived (few days) isotopes studied so far.

Mass transport of oxygen and corrosion products in LBE cooled systems

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Abstract

The Belgian Nuclear Research Centre (SCK•CEN) is a worldwide pioneer in the development of MYRRHA, the first research Accelerator Driven System (ADS). A unique feature of MYRRHA is the use of liquid lead-bismuth eutectic (LBE) as the primary coolant. Use of LBE has many technical and safety advantages. However it is well-known that accurate control of LBE chemistry is a key issue for the design of reliable LBE cooled systems. In the presented research topic the formation, transport and deposition of solid impurity particles during operation of LBE cooled systems are studied as these can result in e.g. clogging of pipes. This fouling problem needs to be mastered for safe operation of MYRRHA and accurate design of filtering systems.

The first part of the research covers the development of a kinetic model for formation of solid lead oxide particles in LBE. A point-kinetic model for the formation of lead oxide in LBE is developed starting from the Classical Nucleation Theory (CNT). CNT predicts the rate of formation of solid nuclei in a liquid phase. Growth of these nuclei is, for the moment, assumed to be mass transfer limited. The point-kinetic model of lead oxide formation and dissolution has been tested in the HELIOS III experimental facility. The theoretical CNT model is corrected based on measurements in stagnant LBE. Using the corrected model, a good agreement between predicted and measured oxygen concentration during formation and dissolution of lead oxide in mixed LBE is observed. The point-kinetic model is extended to account for concentration and temperature inhomogeneities by coupling the chemical kinetics of oxide formation to a Computational Fluid Dynamics (CFD) code, Ansys Fluent. CFD simulations are performed to determine the hydrodynamics of LBE in regions where oxide formation is present. Reynolds Averaged Navier-Stokes (RANS) modeling is used in all computations. The solid oxide particles are modeled as a pseudo-continuous phase (Eulerian framework), using the 'Kinetic Theory of Granular Flow' (KTGF) to account for particle-flow interaction. The particle size distribution is accounted for using Population Balance Equations/ Models (PBE/PBM). An experimental campaign is conducted in the MEXICO LBE loop at SCK•CEN to validate the obtained results of the kinetic model coupled with CFD calculations. Results indicate that the nucleation and growth of large amounts of sub-micron particles of lead-oxide is indeed the dominant mechanism of lead-oxide formation. Qualitative agreement between the model and experimental measurements is obtained by comparison of the oxygen concentration and filter pressure drop.

Current and future work focuses on the description and model development of PbO deposition on heat exchanger surfaces and filter media. The previous treatment of PbO formation is being extended to account for particle attachment and/or surface formation. The combination of bulk oxide formation and surface effects completes the treatment of PbO formation for safety evaluations and development of filtration methods.

Modelling of drying shrinkage in concrete; a multiscale pore-network approach

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Abstract

Volume change is one of the most detrimental properties of concrete, which affects its long-term strength and durability. To the practical engineer, the aspect of volume change in concrete is important from the point of view that it causes unsightly cracks in concrete. Drying shrinkage is one of these volumetric strains, which is defined as the contracting of a hardened concrete mixture due to the loss of water. This contraction causes an increase in tensile stress, which may lead tohttp://www.engr.psu.edu/ce/courses/ce584/concrete/library/cracking/dryshrinkage/DRYSHRINKAGEMAIN-HTML/LINKS-HTML/Shrinkage Cracking.htm cracking. As its definition implies drying shrinkage is highly dependent on water content and hygric properties of the material. The hygric properties of porous building materials can be numerically simulated from their pore structure information.

Many existing models use a common approach for computing drying shrinkage strain, which is based on empirical coefficients obtained through experimental data. However, in this research an approach for modelling of drying shrinkage of cementitious materials is presented via the use of pore network model. This approach is being developed within a multiscale framework in which the pore network model is used to capture the microstructure of the porous matrix in an averaged sense.

In this regard, in first step a pore network model is developed to capture the moisture properties of the material. The output of the pore network model will be used in a continuum framework to predict the drying shrinkage.

Age-related biological effects of dental cone-beam CT exposure

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Abstract

Cone Beam Computed Tomography (CBCT) is a radiographic tool for diagnosis, treatment planning, follow-up and research in dental practice, mostly used in pediatric orthodontics. Although it is considered a low dose imaging modality, it is uncertain that using CBCT is completely risk-free. Investigating low dose effects is of particular interest in pediatric CBCT exposure, since children are more radiosensitive than adults.

As part of the OPERRA-funded DIMITRA project the potential biological effects of CBCT on both in vitro and ex vivo samples were investigated. The main focus was on pediatric patients, but adult samples were included to check for age-related effects. In vitro low dose X-radiation-induced (0, 5, 10, 20, 50 and 100 mGy) effects were studied in stem cells from the apical papilla, dental pulp stem cells and dental follicle stem cells from three pediatric donors. DNA damage and repair kinetics were analysed by microscopical visualization of DNA double strand break (DSB) markers (γH2AX/53BP1) 30 min, 1 h, 4 h and 24 h post-irradiation (p.i.). Ex vivo, DNA damage and repair kinetics were analyzed by microscopical visualization of γH2AX/53BP1 in exfoliated oral mucosal cells collected just before and after (30 min and 24 h) CBCT exposure. Saliva was used to detect local changes in oxidative stress levels (8-OHdG and total antioxidant capacity) induced by CBCT in the oropharyngeal region and salivary glands. Sample collection occurred just before and 30 min after CBCT exposure.

Preliminary in vitro data show that there is a dose dependent increase in the amount of DNA DSBs 30 min and 1 h p.i. for doses higher than 20 mGy. This damage is resolved 24 h p.i... DNA damage analysis in oral mucosal cells reveals that no significant increases in the amount of DSBs can be detected after CBCT examination. The amount of DSBs is significantly higher in children than in adults before and 30 min after CBCT exposure. Data from adult patients shows that salivary 8-OHdG levels do not significantly increase after CBCT examination. The salivary antioxidant capacity, however, decreases significantly in adults. Results from pediatric patients show a significant increase in the amount of 8-OHdG after CBCT exposure and, contrary to adult patients, a significant increase in total antioxidant capacity.

In conclusion, preliminary data indicate that low dose X-rays induce increases in DNA damage in vitro, but CBCT examination does not lead to increased DNA damage in oral mucosal cells. In addition, pediatric patients show increased salivary 8-OHdG levels after CBCT examination combined with a slightly increased total antioxidant capacity, whereas adults show a decreased total antioxidant capacity. These data indicate that adults and children react differently to CBCT exposure. By gaining more insight into the biological effects following CBCT exposure current guidelines for CBCT imaging can be adapted, leading to an improved radiation protection of the patient.

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A hybrid Krylov-balanced Truncation model reduction technique

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Abstract

Near-range atmospheric dispersion calculations are important for improving the safety in and around a nuclear facility. Therefore, the development of a CFD atmospheric dispersion model for the near range was initiated at the SCK - KU Leuven (PhD L. Vervecken, 2015). In this preceding research, Krylov subspace projection was used as model reduction technique to obtain a so called reduced order model (ROM). The performed Doel case study illustrated that the CFD solution, which was produced by an eight million order model, could be reconstructed accurately by the associated ROM of order 100. It turned out that this ROM runs 25 times faster than real time.

In case of an emergency situation, the ROM must also be capable of making a dose assessment and source reconstruction in the least possible amount of time. Therefore, the order of the ROM should be made as small as possible such that its accuracy is still competitive with the CFD solution, but the run time is in the order of (mili)seconds rather than hours. In this regard the Krylov model reduction is already quite an improvement. The aim is to even further optimize the Krylov model reduction by combining it with a Balanced Truncation model reduction technique.

^{137}Cs sorption on glauconite sands of the Neogene

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Abstract

A good understanding of the processes and mechanisms controlling radionuclide transport in the barriers surrounding repositories for radioactive waste is crucial. The Neogene glauconite sands[1] are a possible complementary sorption sink in the sandy embankment of the surface disposal facility for low and intermediate short lived radioactive wastes. Additionally in the concept of geological disposal in the Boom Clay or Ypresian clays, glauconite sands might act as an additional sorption sink.

The aim of this research is to study the sorption behavior of a set of radionuclides on the glauconite sands. In this first phase the research focused on sorption behavior of ^{137}cesium (Cs) and more specific on the sorption potential, the effect of the morphology on sorption of ^{137}Cs and the in situ sorption of the glauconite sands.

A set of sands were selected from different depths in the Neogene sedimentary succession. The Radiocesium Interception Potential (RIP) protocol was used in batch experiments to eliminate the competition of Cs with comparable cations (e.g. Potassium (K), ammonium (NH_4^+)). Initial test showed a high sorption potential (log K_d 3.2 to 3.6 at 0.5 mM K) for ^{137}Cs on the glauconite sands, with the sorption potential proportional to the percentage of glauconite present in the sand. Comparing the results of different glauconite pellet sizes indicate a small increase of sorption potential with decreasing glauconite pellet size. However the sorption potential does not represent the in situ sorption. To obtain the in situ sorption the K concentration in the pore water has to be taken into account. This leads to a significantly lower in situ sorption (Log K_d 2.2 to 3.2). Nevertheless, based on this information glauconite could be a good sorption sink for ^{137}Cs.

However, to thoroughly assess the glauconite sands as a sorption sink, future research needs to focus on the kinetics of the Cs sorption and the effect of the different stages of weathering on the Cs sorption potential.

[1] Sands of Neogene age (23 to 2.5 million years ago) containing up to 80 wt% glauconite, mostly in the form of pellets (on average 600 – 100 µm).

Polydispersity and polyfunctionality of Boom clay dissolved organic matter

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Abstract

In Belgium, Boom Clay (BC) is investigated as a potential host rock for the geological disposal of radioactive waste. An important issue concerns the mobility of uranium, as it represents the most abundant radionuclide in nuclear waste. In order to complete a model of uranium mobility in Boom Clay, all factors concerning clay-radionuclide interactions should be taken into account. Based on previous research, Boom Clay contains significant amount of organic matter – particulate and dissolved. This dissolved organic matter (DOM) plays a critical role in uranium mobility in the porous medias since it can be involved in the complexation or colloidal formation processes. The DOM is very heterogeneous both from a chemical and from a physical point of view. From one hand, it is polydisperse, containing species ranging from hundreds Dalton up to hundred thousand Dalton. From the other hand, it is polyfunctional, i.e. characterised by the presence of several functional groups with labile protons such as carboxylic groups, phenolic groups and amines. Polydispersity and polyfunctionality of organic molecules effects the DOM binding properties towards radionuclides, e.g. uranium. The aim of this work is to investigate the influence of physical and chemical properties of Boom Clay DOM on its interaction with uranium (VI).
Firstly, in order to investigate the effect of polydispersity and polyfunctionality of DOM on complexation and/or colloidal formation with U(VI), the Boom Clay DOM must be extensively characterised.

Different samples of Boom Clay DOM are obtained using either piezometers in the HADES underground facility or leaching from 'peeled' Boom Clay core from the same site. Firstly, the separation of various size fractions performed without oxygen access using ultrafiltration technique. The separation of humic acid from BC DOM fraction performed by precipitation at pH=2. Then, the concentration and size distribution are measured by several methods, e.g. size-exclusion chromatography (SEC), carbon analysis (TOC) and ultraviolet-visible spectrophotometry (UV-VIS). Furthermore, the naturally-occurring elements associated with different fractions are analysed by ICP-MS. The polyfunctionality of Boom Clay DOM fractions is characterised using X-Ray Photoelectron spectroscopy.

The hippocampus: a target for premature aging after early-life irradiation

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Abstract

The human developing brain is highly sensitive to ionizing radiation exposure [1]. Follow-up studies of atomic bomb survivors in Hiroshima and Nagasaki [2] and pediatric patients receiving cranial radiotherapy, have reported cognitive defects at adult age, respectively after pre- and postnatal irradiation exposure. The latter even suggested the presence of Alzheimer's disease (AD) hallmarks long after receiving radiotherapy [3, 4]. The long-term radiation-induced changes show a remarkable similarity with age-related hallmarks, including reduced neurogenesis, neuro-inflammation, oxidative stress and DNA damage. Still, the mechanisms underlying the radiation-induced defects to the developing brain remain poorly understood. Previous investigations in our laboratory have convincingly identified the hippocampus as a prime target for radiation-induced defects to the developing brain. Following prenatal irradiation with 1-Gy X-rays, an aberrant neurogenesis in the hippocampal dentate gyrus and a reduction in hippocampal long-term potentiation was noted in adult C57BL/6J mice. This radiation-induced hippocampal impairment was confirmed in 90-week old mice that had been prenatally irradiated, by a clear decrease in hippocampal volume and impaired hippocampal-dependent cognition. Our current goal is to evaluate hippocampal dysfunctionality after early-life irradiation, possibly leading to accelerated brain aging and AD pathology. To this end, we optimized an *in vitro* aging model using primary mouse hippocampal neurons. Maturing neurons will be irradiated with 1.8-Gy X-rays, after which the effect on cellular aging will be established by examining neuronal connectivity, senescence, amyloid beta (Aβ) and p-tau depositions, etc. This *in vitro* model will be complemented with *in vivo* studies using triple transgenic (3xTg-AD) mice predisposed to developing AD and showing accelerated aging. After 1.8-Gy irradiation of ten-day-old 3xTg-AD mice, cellular aging and AD pathology will be investigated with a focus on the hippocampal region. In all, our results will give better insights into possible radiation-induced aging and neurodegeneration after X-ray exposure to the developing brain, which will ensure a better protection of the unborn child and a better follow-up of children receiving cranial radiotherapy.

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Foliar uptake of Cs^{137} by spinach at different growth stages: experimental setup and preliminary data on interception fractions

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Start date as PhD: November 1st, 2016

Abstract

Radionuclides present in the environment can enter the human food chain through uptake by agricultural plants leading to possible human exposure to radiation. Currently, large uncertainties still exist, associated with the contamination of food crops via the foliar pathway. Hence, it is of basic importance to produce data on the main processes involved in order to improve the current modelling approaches. The main processes governing the foliar uptake include the interception of wet deposition by canopy which is the one studied in this work. We experimentally simulated an acute contamination of spinach leaves considering different stages of plant development: 4-5 true leaves (Stage I); 6-8 true leaves (Stage II); 10-12 true leaves (Stage III). Plants were grown in hydroponic system and simulated irrigation water containing 75 kBq of Cs^{137} (in the form of CsCl) was applied to spinach crops under controlled environmental conditions. First, both the growing and the contamination setups were optimized. Specifically, the optimal plant growing conditions were found in terms of nutrient solution composition, concentration and pH; air temperature (T) and humidity (RH); growing medium; plant support; photoperiod (light hours per day); and light intensity. Related to the contamination system, single boxes 36 cm x 45.5 cm x 36 cm were used to simulate the sprinkling of the plants and a multilayer system was applied to prevent the contamination of the root compartment. The system optimization resulted in low values of the standard errors of any collected data ensuring reliable interception fraction calculations.
The interception fraction f is defined as the activity intercepted by the leaves divided by the total activity deposited. In the sprayed spinach plants, it ranged from 21.40 % (n=6, s.e.=0.007) at the Stage II to 36.64 % (n=7, s.e.=0.016) at the Stage III, hence, increasing with the growth stage according to the increase of biomass and leaf area. The mass interception fraction fB, defined as the ratio between f and B with B dry biomass per unit area, was about 49 m^2 kg at the Stage II and reached 29 m^2 kg at the stage III. The same decreasing trend was shown by Choi et al. (2001) while studying the uptake and translocation of radiocesium by radish plants. The LAI normalized interception fraction fLAI was obtained by dividing the interception fraction by the LAI. The LAI is the area - one side measured - of the leaf surface per unit ground area and the values of fLAI ranged from 3.7 to 4 from Stage II to Stage III with a standard error of 0.14 and 0.15 respectively. The results obtained seem to suggest that the above biomass is a more certain variable in the prediction of interception fractions than the LAI as also found by Bengtsson et al. (2014). Further experiments will be performed to confirm these preliminary results and test whether the biomass could be a accurate parameter to predict, among others, the interception fraction of Cs^{137}. Additionally, plant features will be investigated via optical and electron microscopy. Stomata and wettability analyses will be carried out to verify (or not) the correlations between interception fraction of wet deposited radiocesium and plant morphological characteristics. In a later phase, these research outcomes will be used to examine the current modelling approaches and propose, if possible, model improvements for a better estimation of the radiocesium interception fraction by spinach crops.

Cytotoxicity assessment of gold nanoparticles on non-cancerous cell lines

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Abstract

Gold nanoparticles (AuNPs) have emerged as promising radiosensitizers, which accumulate in the tumor and increase the effectiveness of external beam radiotherapy by local production of reactive oxygen species (ROS) and secondary electrons. At UNamur, 5-nm gold nanoparticles coated with an organic shell of polyallylamine are produced by plasma vapour deposition (AuNPs@PPAA). Optionally, the AuNPs@PPAA can be conjugated to anti-EGFR antibodies (Cetuximab) (Ctxb-AuNPs@PPAA) which actively target EGFR-overexpressing cancer cells *in vitro* and *in vivo*. However, *in vivo* biodistribution studies have demonstrated a significant accumulation of Ctxb-AuNPs@PPAA in liver and spleen. Therefore, the cytotoxicity profile of the gold nanoparticles should be investigated properly in healthy cell types prior to the use in clinical applications.
Human kidney (HK-2) cells and telomerase-immortalized microvascular endothelial (TIME) cells were studied as first examples of healthy cells. We performed MTS tetrazolium cytotoxicity assays and live cell imaging with apoptotic markers Annexin V and caspase 3/7 after 3 and up to 72 hours of incubation with (Ctxb)-AuNPs@PPAA, respectively. The gold concentrations tested ranged from 0.001 mg/ml to 0.05 mg/ml.
The MTS cytotoxicity assay resulted in a significant dose-dependent reduction of cell viability in TIME cells. In contrast, an increased tetrazolium-to-formazan conversion was seen in HK-2 cells. Conjugation of Cetuximab to AuNPs@PPAA did not increase cytotoxicity *in vitro* after 3 hours of incubation compared to AuNPs@PPAA. Live cell imaging with a concentration of 0.05 mg/ml of gold showed a significant increase of Annexin V and caspase 3/7 signaling after 8 and 10 hours of incubation in TIME and HK-2 cells, respectively. Lower concentrations, even down to 0.003 mg/ml, resulted to apoptosis in TIME cells after longer incubation times (60h).
In the future, we will assess the cellular (Ctxb)-AuNPs@PPAA uptake by means of ICP-MS and TEM. Oxidative stress induced by exposure to (Ctxb)-AuNPs@PPAA will by evaluated by means of ROS measurements. Finally, the toxicity evaluation will be completed with studies testing a liver cell line.

Acknowledgements
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Towards Bismuth-213 labeled nanobodies, a new treatment approach in Targeted Alpha Therapy

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Abstract

The use of nanobodies (Nbs) as vehicles in targeted alpha therapy (TAT) has gained traction due to their excellent in vivo properties, high affinity and specificity, fast diffusion and clearance kinetics. Moreover, Nbs show good tumor penetration due to their small size. The main strength of TAT is the potential to deliver a high level of ionizing radiation in a localized manner because of the short range of alpha particles in tissue. In combination with a tumor-seeking vehicle, TAT could specifically eliminate isolated cancer cells, while causing little damage to healthy cells. The aim of this study is to develop a novel molecular targeted therapy that combines the α-particle emitting radioisotope bismuth-213 (^{213}Bi) and the HER2-targeting 2Rs15d-Nb to selectively destroy HER2-positive metastases.

In a first step, a separation method was developed to produce pure ^{213}Bi. From an onsite thorium-229 (^{229}Th) source, the purified actinium-225 (^{225}Ac) is loaded on a pre-packed column containing AG MP-50 cation exchange resin. In dilute acid, both ^{225}Ac and ^{213}Bi in their stable 3+ oxidation state are efficiently adsorbed on this cation exchange resin. ^{213}Bi is selectively eluted from the cation exchange resin as anionic BiI_4^-/BiI_5^{2-} species. Chemical separation experiments were performed on non-radioactive solutions (were lanthanium (La) was used as simulant for Ac) to develop a reliable Ac/Bi separation methodology which was later applied on radioactive ^{225}Ac. Different bed volumes and eluents concentrations were evaluated. Inductively-coupled plasma mass spectrometry (ICP-MS) was used to evaluate the performance of the separation methodology. Our final aim is to produce high purity ^{213}Bi and minimize ^{225}Ac breakthrough.

In a second step, ^{213}Bi-labeled HER2-targeting Nbs were developed. For labeling purposes the diethylenetriaminepentaacetic acid (DTPA) derivative was selected as bifunctional chelator due to its high Bi complexation properties. DTPA-anti-HER2 Nbs were synthetized and purified. Radiolabeling experiments of ^{213}Bi-DTPA-anti-HER2 Nbs were performed showing high radiochemical labeling yields. Due to the 46 min half-life of ^{213}Bi, the ^{213}Bi labeling reaction and quality control of ^{213}Bi preparations must be performed in a very short time frame to avoid significant decay losses. As such, optimization of the labeling strategy is essential to maximize the overall yield. The ^{213}Bi-labeled 2Rs15d-Nb will be evaluated for their stability, binding specificity and immunoreactivity in $HER2^{pos}$ SKOV-3 cells.

Differences in radio sensitivity to gamma radiation between rice and Arabidopsis

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Abstract

Understanding plant radiosensitivity is an important element to consider in order to provide more insight into responses of plants to gamma radiation. According to the UNSCEAR 2008 report, several factors influence this radiosensitivity namely: the plant species, the growth stage of the plant and the genome size. In this study, two plant species reported to differ in radiosensitivity were used: rice (*Oryza sativa cv. Nipponbare*) and arabidopsis (*Arabidopsis thaliana Col-0*). The former is considered to be more radiosensitive due to its large complex genome compared to the latter. Both plants were exposed to four gamma dose rates and analysed for effects at different levels of biological complexity (growth, enzyme activities and molecular level). Previous studies on arabidopsis measured the effect of gamma radiation on antioxidative enzymes activities immediately after gamma exposure. Therefore, the same analyses were carried out in rice to enable the comparison of both plants. These plants were also allowed to recover for two weeks after which the same parameters were analysed as mentioned above. Growth measurements in rice after two weeks of irradiation revealed a decrease in plant height in exposed plants compared to controls. This decline was even more pronounced after two weeks of recovery. In arabidopsis, the effect on growth was determined by measuring the height of the inflorescence stem in recovery plants and this was found to increase significantly at all dose rates compared to the controls. There were no differences in total fresh weight measured in rice immediately after irradiation but this significantly declined in exposed plants following recovery. Conversely, in arabidopsis there was a significant increase in total fresh weight in irradiated plants. This trend was also observed in the recovery plants except at the highest dose rate where the fresh weight was not significantly different from the controls. These growth responses suggest that gamma radiation had a hormesis-like effect in arabidopsis but not in rice. Further comparisons were made at the enzyme level more specifically on the activity of different antioxidative enzymes. For arabidopsis, *van de Walle et al (2016)* observed a significant induction in syringaldazine peroxidase (SPX) and guaicol peroxidase (GPX) activities in shoots and roots repsectively. In contrast, we found no significant difference in SPX activity in rice shoots whereas rice roots showed a significant decline in GPX activity. Ascorbate peroxidase (APX) activity significantly declined in gamma exposed rice shoots, while there was no induction of the APX activity in arabidopsis shoots. This decline in antioxidative enzyme activity in rice instead of the expected increase as seen in arabidopsis is an indication that rice plants cannot deal with enhanced reactive oxygen species (ROS) production or may be using different mechanisms to deal with oxidative stress following gamma irradiation. Taken together with the decreased growth, the decline in antioxidative enzyme activity in rice in response to gamma radiation is an indication of rice being more radiosensitive than arabidopsis.

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Direct sampling VS our new multiphase-multiresolution simulated annealing approach: which porous media reconstruction looks best?

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Abstract

The microstructure of a radioactive waste confinement barrier strongly influences its flow and transport properties. Numerical flow and transport simulations for these porous media at the pore scale are necessary for in-depth understanding of the pore-scale processes, and might for instance allow making predictions beyond current experimental timescales. Such simulations of course require input data that describe the microstructure as accurately as possible. This data can be deduced from various imaging techniques, but for complex systems, a combination of techniques is required. To merge all available information into a single synthetic but realistic microstructure, and to lower the need for *e.g.* costly 3D images, high quality numerical reconstructions are needed. Simulated annealing (SA), which is based on structural descriptors, is one of the oldest approaches, but has recently received a lot of attention. The method is typically only applied to binary images and is computationally very demanding without optimized algorithms and inventive computational approaches. We extended the state-of-the-art of the SA approach to multiphase reconstructions, due to a decrease in computational burden through the use of a multiresolution-multiphase hierarchical approach. The method performs the reconstruction by first simulating a binary image at the coarse resolution and refining it afterwards. Once the simulation of the first phase is finished, the corresponding pixels are frozen and the next phase is reconstructed. This new methodology reduces the computational time by at least 50% compared to single grid simulations while additionally improving the reconstruction quality. In reconstruction with a high particle size to simulation grid dimension ratio, the speed up can be several orders of magnitude.
Compared to Direct Sampling (DS), the new SA algorithm does not show the problem of honouring the histogram and the occurrence of verbatim copies. Additionally, the new SA algorithm shows an improvement in the long range connectivity of the different phases within the training image. We show this using two case studies: Cement paste and Boom Clay.

Uranium isotopic composition determination using CdZnTe and $LaBr_3$ detectors

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Abstract

In recent years there has been an increased interest in using medium resolution detectors of the CdZnTe (CZT) and $LaBr_3$ types for the determination of isotopic composition of uranium and plutonium bearing materials. Unlike HPGe detectors, these detectors do not require cooling for their operation and due to their compact size and attractive features are a promising alternative to HPGe.

To determine the isotopic composition a specialized algorithm is required. Such algorithms are very well developed for HPGe detectors and are available as commercial products[1,2], however as for the CZT and $LaBr_3$ detectors there is no such an adequate analysis tool for uranium and plutonium spectra measured with medium resolution quality. Due to significant differences in resolution, response functions and statistical criteria, the HPGe detector algorithms cannot be directly applied to medium resolution quality spectra. However, the net peak area based concept used in algorithms for the isotopic composition determination with HPGe detectors can be modified in such a way to account for the particularities of medium resolution quality spectra.

The main goal of this PhD project is to develop an isotopic composition determination algorithm(s) particularly suited for CZT and $LaBr_3$ detectors. To determine the possibilities, limits and the uncertainty budget of the developed algorithm(s) a quantitative assessment of their performance in a variety of measurement conditions is required.

The current poster reports on the results of uranium isotopic composition determination algorithm developed for CZT and $LaBr_3$ detectors with the necessary modifications. Tests were conducted on uranium spectra of certified standards (CBNM) with ^{235}U enrichment varying from 0.31% to 4.46%. The results revealed the possibility to use the net peak area based algorithm for uranium isotopic composition determination on CZT and $LaBr_3$ detectors, although certain limitations were discovered.

Acknowledgements
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Internal gelation process for the production of simulated transmutation fuel particles

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Abstract

In any advanced nuclear fuel cycle, partitioning and transmutation (P&T) is a key strategy to reduce spent nuclear fuel's radiotoxicity and heat generation: Long-lived minor actinides (MA) are partitioned from spent nuclear fuel and subsequently converted to manufacture dedicated fuel pins or targets. These are used as nuclear fuel in fast reactor systems where the actinides are fissioned to short-lived radioisotopes.

An essential link between the partitioning and the transmutation is the conversion of the separated minor actinides into solid precursors to fabricate fresh fuel suitable for minor actinide recycling. Among transmutation fuels, particle fuel (*Sphere-Pac* fuel strategy [1]) offers certain beneficial properties compared to pellet fuel. Particles can be prepared without any formation of dust via an aqueous synthesis pathway. Moreover, the fuel manufacturing process offers advantages in terms of automation up to and including the rod filling step. Strategies to fulfil this task are sol-gel processes, where a stable solution containing the desired metals, the *sol*, is converted into a solid gel [2].

The focus of this PhD study within the first year was the production of lanthanide-doped UO_2 microspheres applying the sol-gel route via internal gelation, where a pH rise driven by the decomposition of an agent in the feed solution triggers the solidification. Nd(III) was used as simulant for the minor actinide Am(III). Cerium will be used in the tetravalent and trivalent state to simulate plutonium and to investigate the influence of the metal's oxidation state on the synthesis process and product.

Feed solutions of $Nd(NO_3)_3$ and $Ce(NO_3)_3$ were characterised by UV/VIS spectroscopy. Pure UO_2 particles and $U_{1-y}Nd_yO_{2\pm x}$ (y = 0.05 – 0.30) particles were prepared by the sol-gel route via internal gelation. The sintering behaviour of the gelled particles was studied by thermogravimetric analysis (TGA) and the crystal structure was analysed via powder X-ray diffraction (XRD).

Ammonium diuranate (ADU) was prepared via the addition of ammonia to a uranyl nitrate solution and a comparison of ADU and the gelled uranium particles was carried out via TGA and XRD. An ADU type crystal structure was found for the gelled uranium particles evolving into U_3O_8 during calcination.

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On the capillarity and micro-structure of hardened cement paste: a multidisciplinary study

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Abstract

The presented study investigates the relationship between microstructure and gas transport in a two-phase flow regime from a macroscopic perspective.
Cementitious materials are integral building blocks in radioactive waste repositories. The material itself is characterized by a complex and dynamically evolving pore structure which governs the transport properties and processes.
Two-phase flow in cementitious materials is considered as a capillary controlled process and, thus, it is a function of interfacial tension, contact angle, pore radius, saturation and wetting-phase distribution. These parameters are compiled in the concept of capillarity, sealing efficiency and effective transport parameters. To provide inside into the two-phase flow regime, this contribution provides preliminary results on the (i) wettability, (ii) capillary sealing, (iii) microstructure and (iv) water distribution of hydrated cement paste which were assessed by means of experimental techniques. Hydrated cement pastes are typically partially water-saturated which affects gas transport and capillary pressure. Since the effect of water on fluid-flow properties is not just directly related to the amount of water (saturation), but also to the distribution of that water in the pore system of cementitious materials gas (N2) physisorption measurements on partially saturated cements were performed. The results reveal that neither capillary condensation below 0.93 P/P^0 is a dominant vapour sorption mechanism nor that simple layer sorption prevails at lower relative pressures pointing out the inapplicability of traditional physisorption models. Contrarily, a surface chemistry controlled cluster-sorption mechanism is proposed which has often been validated for engineered materials like black carbons. The wettability of a solid is quantified by the contact angle (θ) which was determined via column wicking experiments. Applying a capillary bundle model yielded average advancing contact angles between 50° and 58° on hydrated cement paste of different age and porosity. In contrast to commonly assumed perfect wetting ($\theta = 0°$), these data suggest less resistance to wetting-phase drainage in the two-phase regime. The capillary sealing capacity was assessed by means of mercury intrusion porosimetry (MIP) and capillary gas breakthrough experiments coupled with nuclear magnetic resonance measurements. MIP-based threshold pressures are only considered as proxies for the actual breakthrough pressure of gas due to methodological shortcomings like omnidirectional intrusion. Direct capillary breakthrough measurements yielded a threshold pressure of 2.4 MPa which is in the range of the MIP derived values(2.3 to 3.1 MPa). At breakthrough the effective gas permeability is three orders of magnitude lower than the absolute permeability of water ($k_{eff} = 4.1E^{-20}$ m^2 vs. $k_{abs} = 7E^{-17}$ m^2). Saturation monitoring by NMR spin-to-spin relaxometry did not show significant changes in water content up to a maximum pressure difference of 102 MPa at which a relative permeability of 0.02 % was calculated ($k_{eff} = 1.05E^{-19}$ m^2). The unexpected conservation of saturation is currently unclear and is considered as a result of a lack in resolution and temperature effects. However, the low transport capacity at maximum pressure difference may imply either a low connectivity across the sample or that the majority of connecting pore throats are too small to be drained.

Characterization of carbonation-induced changes in roughness of crack surfaces in hardened cement pastes

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Abstract

Cementitious materials are widely used in nuclear applications, for instance in various constructions, containment barriers and waste disposal to prevent release of radioactivity for longer time periods. Hence, the concrete performance becomes a highly important issue and requires detailed studying of deterioration mechanisms. Carbonation is one of such reactions, which results in chemical and physical changes of cementitious materials (lower pH, increased internal stresses, shrinkage, changes in porosity, permeability and diffusivity, altered mineralogy and bulk density). At the same time, physical properties of cementitious materials influence the rate of geochemical processes, especially carbonation rate is faster if the material is cracked. However the exact effect of microcracks on carbonation rate and the consequences of carbonation in cracked material remain unexplored. Understanding the interplay between carbonation and crack properties is required for further simulations and estimation of the concrete durability.

One of the questions is to study how crack properties are affected by carbonation at the pore-scale. The geometry of crack surfaces alters during reaction and changes of surface roughness should be captured experimentally, analyzed and simulated for better understanding of carbonation reaction. Surface topography plays an important role in crack characterization since it influences the transport properties inside the crack. Surfaces with different roughness were obtained by polishing and were examined with the profilometer (in collaboration with VITO), which is the effective technique to measure surface topography at microscale. In this work the experimental results and statistical analysis are discussed. The study showed interesting results on surface roughness change due to carbonation. We may conclude that carbonation of surfaces with high roughness leads to smoothing and such effect can be explained by precipitation-dissolution mechanisms. On the contrary, smoother surfaces did not change much after carbonation, but vertical movements of areas near microcracks were observed, which is a possible consequence of increased solid volume under the surface. These results provide us a glimpse on the interconnection between carbonation reaction and crack properties, so the further experimental examination and model development will follow that will help us to answer questions about the effect of rough surfaces on carbonation rate, the effect of carbonation reaction on angle and amplitude of pits at rough surfaces, identification of hydrated cement phases that lead to the most significant changes in surface roughness and others.

On-line coupling of HPLC with ICP-MS for elemental and isotopic analysis of spent nuclear fuel

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Abstract

Spent nuclear fuel characterization has always been of crucial importance in nuclear reactor facilities. When it comes to determination of the burnup value of spent fuel samples, accurate and precise measurement of the isotopic composition of U, Pu and Nd is essential [1]. Although thermal ionisation mass spectrometry (TIMS) has long been the benchmark technique for isotopic composition measurement, this project explores the use of sector-field inductively coupled plasma mass-spectrometry (SF-ICP-MS) instead. In contrast to TIMS, SF-ICP-MS can be hyphenated with other techniques, eg. high performance liquid chromatography (HPLC), thereby allowing automated on-line separation of analytes [2] in order to prevent spectral overlap of isobaric nuclides. In addition, HPLC-SF-ICP-MS also offers rapid and effective measurement of multiple analytes within a single analysis [3]. First results of on-line separated lanthanide standards will be presented, as well as an overview of analytical challenges involved in further optimization of an HPLC-SF-ICP-MS method which yields the best obtainable limits of detection, accuracy and precision for determination of actinide and lanthanide isotopic compositions (primarily Nd, U & Pu). More specifically, concerning parameters of HPLC separation, eluent flow rate(s) and composition, column type etc., will be investigated [4]. Application of SF-ICP-MS, on the other hand, requires optimization of both data acquisition (the number of isotopes monitored per run, dwell time, replicates, integration window etc.) and experimental parameters (calibration method and method(s) to correct for mass discrimination). Finally, isotope ratio measurement uncertainties, determined at a later stage, will allow the HPLC-SF-ICP-MS method to be evaluated against TIMS.

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Chemical compatibility of select MAX phases with static Lead-Bismuth Eutectic (LBE)

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Abstract

Nanolaminated ternary carbides, widely known as MAX phases, are considered as candidate materials for nuclear applications due to their remarkable combination of properties, such as thermal/electrical conductivity, thermal shock resistance, machinability, damage and irradiation tolerance, oxidation and corrosion resistance, etc. Their potential use in heavy liquid metal-cooled nuclear systems, such as the ADS irradiation facility MYRRHA and Gen-IV lead-fast reactors (LFRs), is particularly appealing in view of the superior resistance of these materials to liquid metal corrosion. The latter was demonstrated at SCK•CEN by means of screening exposures of various MAX phases (Ti_3SiC_2, Ti_2AlC, Nb_2AlC, Nb_4AlC_3, $(Nb,Zr)_4AlC_3$) to oxygen-poor ([O] < 10^{-10} mass%) static LBE at 500°C for up to 3500 hours; these tests showed no interaction between MAX phases and liquid LBE, indicating the inherent resistance of these materials to LBE dissolution attack. In continuation of that work, the chemical compatibility of Zr-based MAX phases with liquid LBE was investigated at SCK•CEN, since Zr-based MAX phases are promising fuel cladding candidate materials for Gen-IV LFRs due to the low neutron cross-section of zirconium (Zr). This work presents preliminary findings from the exploratory exposure of Zr-based MAX phases (Zr_2AlC, $(Zr,Ti)_2AlC$, $(Zr,Ti)_3AlC_2$) to oxygen-poor ([O] < 10^{-9} mass%) static LBE at 500°C for 1000 hours. Compositional changes were observed locally in the exposed materials, indicating a certain reactivity between LBE and the MAX phase-based materials. For example, the chemical interaction between LBE and Zr_2AlC resulted in the *in situ* formation of $Zr_2(Al,Pb,Bi)C$ solid solutions, due to the intercalation of Pb and Bi atoms into the nanolaminated MAX phase crystal structure. This interaction mechanism was studied by scanning electron microscopy/energy-dispersive X-ray spectroscopy (SEM/EDS), electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM), and the obtained results are discussed here.

Defect clustering and long-range ordening in UO2+x and higher valence phases

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Abstract

Thermal, mechanical and diffusion properties in material are known to be affected by the presence of defects in materials, being point defects or extended defects – 1D defects like dislocations, 2D defects like free surfaces or grain boundaries, or 3D defects like defect clusters. The objective of this PhD is to investigate these material changes by mean of atomistic computer simulations, and to assess how the migration of relevant fission product, in terms of fuel performance and of safety, is affected.

The first stage of this PhD is dedicated to the defect model of UO_{2+x}, where earlier studies have revealed that the defect model is quite complex and involves the formation of interstitial clusters. The charge of these defects is usually compensated by a valance shift of uranium atoms from U(+IV) to U(+V) or U(+VI) depending on the oxygen fraction. Although point defects in UO_2 have been already studied using classical semi-empirical potentials [1] or density function theory [2-3], a complete picture is still missing. In this the present work, the stable arrangement of these valanced U atoms around oxygen interstitials and oxygen interstitial clusters was investigated by mean of classical molecular dynamics calculations and energy minimization schemes, with the LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator) code. Atom interactions are described as a combination of long-range Coulombic interactions with short-range pair interactions and rely on the Buckingham-Morse type developed by [4].
The simulations, performed on a system of about 1000 atoms, were then coupled to genetic algorithms in order to investigate the relative stability of various U(+V) defect arrangement around the oxygen interstitial defects (isolated point defects or clusters). We confirmed the preferential binding of U(+V) atoms with oxygen interstitial compared to a situation where point defects are not interacting; a situation, which could be expected in view of the respective charges of defects. Interestingly, the most stable configuration is not predicted for two U(+V) defects located as first neighbour of the oxygen interstitial, but rather when they occupy second nearest neighbour positions. (see Fig. 1) This study is currently extended towards more complex defect clusters, in order to derive similar results on the stable arrangement of U(+V) defects around such clusters. The study will then address phases of higher oxidation, like U_4O_{9-y} and U_3O_7, in support to on-going experimental work in our laboratories.

Characterization of 24% cold worked DIN 1.4970 steel after ageing

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Start date as PhD: October 1st, 2015

Abstract

With renewed interest in fast spectrum reactors, research in swelling resistant stabilized austenitic stainless steels for use as fuel cladding is being revived after years of standstill. Despite the vast amounts of experimental work conducted between 1970-1990 on the microstructure and mechanical properties of these steels, many questions remain that can be addressed with modern characterization techniques.

For the fuel cladding of the MYRRHA reactor in development at SCK-CEN, a new heat of cold worked DIN 1.4970 (part of the 15-15Ti family) steel was recently produced at Sandvik [1]. In this steel, under certain thermal and irradiation conditions, TiC nanoprecipitates form on dislocations (see Figure 1). These precipitates stabilize the dislocation network and serve as vacancy-interstitial recombination centers, which improves the creep resistance and reduces irradiation swelling respectively [2]. The low operating temperatures (~400°C) envisaged for the MYRRHA reactor, may inhibit precipitation of TiC [3]. Therefore, a thermal ageing heat treatment at elevated temperature may be required.

However, during such heat treatment, undesirable processes such as recrystallization and partial or complete recovery of the cold work may also take place. This could negatively impact mechanical properties and radiation resistance.

In this work, cold worked DIN 1.4970 steel was subjected to different ageing heat treatments between 500 and 1000 °C. The resultant microstructure was investigated with LOM, SEM, EBSD and TEM to elucidate recrystallization, recovery, and precipitation behavior. Size, distribution and orientation of precipitates were studied in thin foils using Dark field imaging, HRTEM, EFTEM, EDX and EELS. New insights were gained about the nanoprecipitate shape and relationship to the matrix using probe corrected HAADF STEM.

References

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Calorimetric studies of the U-Mn and U-Al binary systems

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Abstract

Under the pressure of international treaties in the frame of non-proliferation, the global civil use of high-enriched uranium is gradually being reduced. A main area to develop low-enriched uranium (LEU) used in civil applications is for the production of fission radioisotopes, in particular for the highly demanded isotope ^{99}Mo. This PhD seeks to develop LEU targets for the production of medical isotopes to conform with international demands.

The first objective undertaken here is to envision new fuels suitable for isotope production and processing. Material design and engineering for medical-isotope production demand high temperature phase stability and thermal property data to assess its viability to withstand normal and critical conditions. High-density intermetallics, such as U_6Mn and U_6Fe, have come into consideration for next generation radio-isotope production targets to increase isotope yield within the same volume of space in a target. However, relatively little calorimetric data is available on these compounds. The present study seeks to extend the material property database for advanced nuclear materials, in particular the U-Mn binary system, so that better targets can be rationally designed.

To realize temperatures and enthalpies of transition for the U-Mn binary system, a series of U_xMn100_{-x} binary alloys have been strategically made to represent every crystallographic and physical transformation of this system. Sample composition and homogeneity was analysed with SEM, EDX, and XRD. Following, a comprehensive characterization of high temperature phase equilibria was performed with differential scanning calorimetry. There are notable similarities and difference with what is reported in literature. The eutectic transformation involving UMn_2 and βMn is found to occur at 1051°C and at 58 wt% Mn with an enthalpy of 125,5±15 J gram^{-1}. U_6Mn is found to incongruently melt at 734°C to γU + liq, in contrast with current diagrams. The enthalpy of this transformation found here is 44.45 J gram^{-1}. Liquidus temperatures are in general found to be in agreement with literature. A revision of the U-Mn phase diagram maybe considered to reflect current calorimetric data.

Developing of the advanced FOCS system for ITER and WEST

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Abstract

The purpose of this work is to develop a diagnostic system to measure plasma current in ITER and WEST tokamaks, based on a fiber optic current sensor (FOCS). This system must satisfy ITER performance requirements and be compatible with the ITER hostile environment. Operation of a FOCS consists in measuring the State of Polarization (SOP) rotation induced by the magnetic field in the optical fiber. Ideally, the rotation of the SOP is directly proportional to the current the sensing fiber encloses. The limitations of the FOCS accuracy are mostly related to the imperfection of the optical fiber and Faraday mirror.
In the previous works modeling of the FOCS performance as function of fiber properties has been done. Later, the influence of temperature on the properties of the fiber (changing of the Verdet constant and the beat length) and the polarimetric imperfection of the Faraday mirror were included in the model. In the present work the simulation model will be extended by including the influence of various effects (such as irradiation) on components of the sensor and it will allow to study the impact of these effects on the total system accuracy.
The Faraday mirror (FM) is one of the key elements of a FOCS. Radiation and temperature impact on the properties of the FM must be taken into account. Assessment of these effects is required for selecting locations of the Faraday mirror in ITER. Measurement of the effect of temperature on the properties of Faraday mirrors started in July of this year. Five different types of FMs were procured and three samples have been measured. Preliminary results show that the mirrors have a big coefficient of dependence of the optimal wavelength on temperature (around -1 nm/°C). Investigation of other mirrors and detailed data analysis is under way. Such an influence may have a significant effect on the operation of the device in general and the design of FOCS, and will be studied in details. It must also be taken into account when designing the irradiation testing. Gamma irradiation induced heating will change the temperature of the sample during the experiment. Hence, all temperature measurements should be done and implemented, before starting of radiation measurements.
Another part of the PhD is the development of Polarization Optical Domain Reflectometry (POTDR) technique for plasma current and distributed magnetic field measurements. A simulation model of the FOCS with POTDR for standard fiber is being extended for the spun fiber case.

Pore pressure estimation in irradiated UMo

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Abstract

In the last decades, most of the research reactors around the world converted their driver fuel from High-Enriched Uranium (HEU) to Low-Enriched Uranium (LEU), adopting uranium silicide. However, this choice was not applicable for high-power research reactors, such as BR2 at SCK•CEN, since it would have led to an excessive loss of performance. Therefore, since the beginning of the century and in collaboration with other research institutes worldwide, SCK•CEN has initiated a deep investigation on U(Mo) dispersion fuel as an alternative LEU based driver fuel for those reactors that needed to preserve very high neutron fluxes. The performed irradiation tests revealed that two main phenomena affect this new fuel concept: the interaction between the U(Mo) fuel particles and the aluminium matrix in which they are dispersed, and the fuel swelling. Different engineering solutions have been proposed and tested to limit these effects, such as silicon or zirconium nitride coating of U(Mo) kernels, and powder annealing. This presentation will deal with the destructive inspections that have been carried out on the SELENIUM 1a fuel plate, the most recent U(Mo) full-size fuel plate irradiated in BR2 in 2014. The fuel microstructure was analysed by means of Scanning Electron Microscopy (SEM). In particular, image analysis was employed to evaluate porosity evolution with burnup to determine the kinetics of the recrystallization effect. A stereological approach was used to reconstruct the 3D features starting from the 2D information derived from SEM pictures. Pore fraction, dimensions and density were estimated in a large fission density range (from 2.3 to 5.5×10^{21} f/cm^3), in order to study the evolution of the pore population during high burn-up structure (HBS) development in U(Mo). Starting from these data, a model has been developed to estimate the pressure of the fission gas bubbles, whose evolution has been interpreted on the basis of irradiation effects on the mechanical properties of the hosting material.

Mechnical properties and fracture surface of baseline and novel tungsten for fusion application

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Abstract

The aim of this research is to establish a reference mechanical database of tungsten materials as assess neutron irradiation effect. To achieve the mechanical properties, mini-tensile test and fracture surface analysis was applied to six types of tungsten based materials. Two commercial grades produced from Europe and China: Plansee ITER grade W (IGP) and AT&M ITER grade W (CEFTR), respectively. As well as, four R&D grades developed by institute from Germany (two particle reinforced tungsten), Czech Republic, and China: W-1 wt% TiC (W1TiC), W-2 wt% Y_2O_3 (W2YO), Ultra Fine Grain W (UFG), and W-0.5 wt% ZrC (W0.5ZC), respectively. To consider the influence of texture after rolling process, two sampling orientations, longitudinal and transverse, were investigated for IGP and CEFTR. Testing temperature of 300ºC, 400ºC, and 600ºC were selected to comply with the operation condition of the water-cooled Diverter of Demonstration Power Plant (DEMO). Although all the materials showed feature of brittle fracture on part of the fracture surface, most of the materials had ductility at 300ºC, except UFG and IGP in transverse orientation. High yield strength and ultimate tensile strength were recorded for CEFTR, W0.5ZC, and W1TiC at 600ºC, which can be considered as promising high temperature performance materials. For CEFTR, transverse orientation revealed higher strength compared with the longitudinal orientation at all testing temperature; however, the Ductile to Brittle Transition Temperature (DBTT) of samples tested in transverse orientation was higher than the one tested in longitudinal orientation.