

Tag der Forschung 2022



25. April 2022, 8:30-16:00 im KKL Besucherzentrum

Agenda

From 8:30	Welcome Coffee	
9:15-9:25	Opening and welcome	Th. Franke, KKL M. Plaschy, swissnuclear
9:25-09:45	ETHZ/EPFL MSc in Nuclear Engineering up- dates and new research directions at ETHZ/PSI	A. Manera, ETH
09:45-10:15	Short presentations on posters (Session 1)	See below
10:15-10:45	Coffee break and Poster Session	
10:45-11:15	PSI INTEGER Research Programme on Material Ageing & Structural Integrity	H.-P. Seifert, PSI
11:15-11:45	Hydrogen Quantification and its Impact on Liner Nuclear Fuel Cladding	L. Duarte, PSI
11:45-12:15	Short presentations on posters (Session 2)	See below
12:15-14:00	Stand-up Lunch and Poster Session	
14:00-14:30	Development in ATF	C. Cozzo, PSI
14:30-15:00	Uncertainty and sensitivity analysis in reactive transport modelling: application to cesium sorption in clay	L. Podofilini, PSI
15:00-15:30	Current status of the GIF Systems and their development in Europe	K. Mikityuk, PSI
15:30-15:45	Closing	M. Plaschy, swissnuclear

Short presentations on posters (Session 1, 09:45-10:15):

- Characterization of Strain Localization under Cyclic Loading through Microscopic Digital Image Correlation, **C. Kursun**
- Development of a crack arrest toughness measurement techniques using small specimens to evaluate the fracture behavior in the ductile-brittle transition region of “ferritic” steel. **P. Gao**
- HyUp “Searching for the causes of increased hydrogen uptake at high burnup in Light water reactors (LWR)” **J. Bertsch**
- Synchrotron X-ray diffraction and spectroscopy for analysis of crystal defects and fission product speciation in irradiated UO₂ fuels, **S. Bhattacharya**
- HyMec “HYMEC – HYdrides & MEchanics”, **O. Yetik**
- Lasso Monte Carlo for Stochastic Uncertainty Quantification in Nuclear Burn-up Calculations, **A. Alba**

Short presentations on posters (Session 2, 11:45-12:15):

- SUBFLOW for Polydisperse Model development (SUPERMO), **Omar Al-Yahia**
- Spent Fuel Pin Neutron Emission Measurement with Scintillators (NEWS), **A. Wolfertz**
- Advanced source term analysis with MELCOR (ASTAM), **T. Lind**
- Hydrodynamic Experiments to Characterize Aerosol Retention (HECTAR), **D. Suckow**
- Numerical prediction of boiling crisis considering surface characteristics, **Y. Sato**
- ATHESC Thermodynamic modelling of CRUD formation phenomena in LWR, **S. Nichenko**

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ETHZ/EPFL MSc in Nuclear Engineering updates and new research directions at ETHZ/PSI

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^bPaul Scherrer Institut

In order to maintain core competences in Switzerland in the field of nuclear engineering, a joint MSc program was developed through a cooperation between EPFL and ETHZ. The program guarantees a steady flow of young engineers to support the continuous operation of nuclear power plants in Switzerland and to develop the know-how needed for the future decommissioning phase.

In the presentation the progress with the joint EPFL/ETHZ MSc included planned updates will be presented. In addition, a brief overview will be given of new research developments at the Paul Scherrer Institut and in the newly funded Laboratory for Nuclear Systems and Multiphase Flows at ETHZ/PSI.

PSI INTEGER Research Programme on Material Ageing & Structural Integrity

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After short introduction on material ageing and its significance for safe long-term operation (LTO) of LWRs, a brief overview on the INTEGER research programme in the Laboratory for Nuclear Materials (LNM) is given. Out of the multitude of activities and excellences, a few selected current or recent R&D activities are presented by the specific and important case of stress corrosion cracking (SCC) in Alloy 182/82 dissimilar metal welds (DMW), which is an ongoing issue in both PWRs and BWRs. This involves the characterization of SCC initiation and growth and generation of data for integrity and lifetime assessment, the mitigation of SCC initiation, integrity assessment in this context, optimization of non-destructive examination for SCC in DMWs or expertise's & services for ENSI and the Swiss utilities. This overview just gives a flavor of our competences and skills. Finally, some potential and newly emerging ageing issues and R&D needs for LTO beyond 50 years are shown.

INTEGER - Safe & Efficient LTO in the Context of Material Ageing

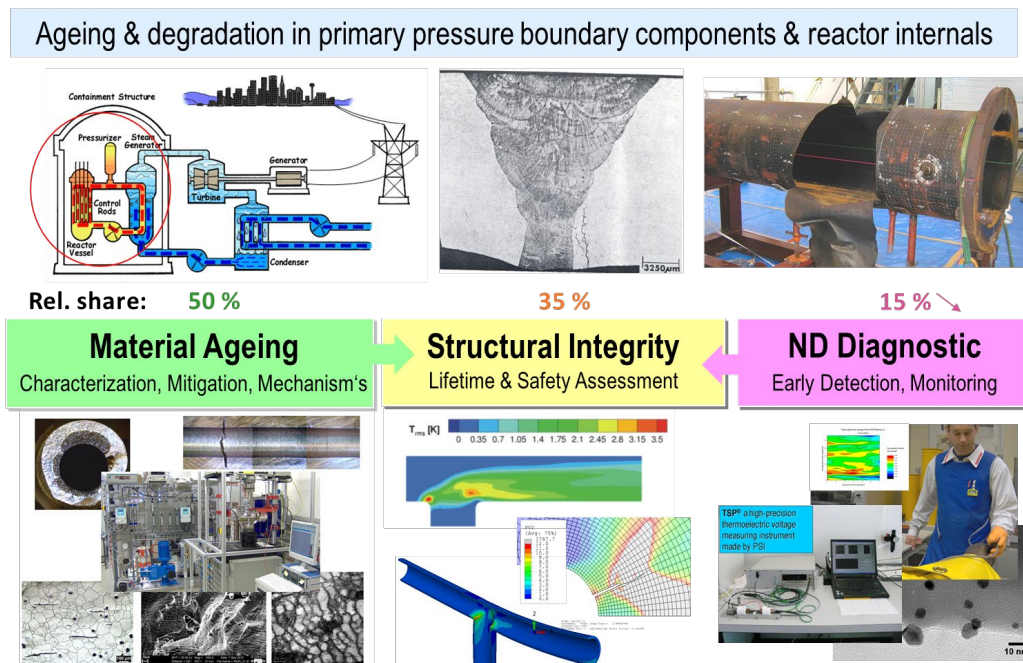


Fig. 1: Overview on INTEGER Research Programme.

Hydrogen Quantification and its Impact on Liner Nuclear Fuel Cladding

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Swiss nuclear power plants use zirconium-based nuclear fuel claddings with liner due to an improved performance. A layer with 70-100 μm thickness of a low-alloyed zirconium is bonded in a metallurgical way by co-extrusion to the inner or outer part of the cladding. While an outer liner improves the cladding corrosion resistance, the inner liner improves the resistance to crack initiation because of pellet-cladding interaction (PCI).

During operation in the reactor, zirconium claddings are subject to water corrosion. From the corrosion mechanism, hydrogen is formed, and a part of it is absorbed and diffuses into the cladding. When the solid solubility is exceeded, hydrides precipitation occurs. These precipitates constitute a factor of risk for the mechanical integrity of the fuel rods due to their brittleness. The risk is increased especially for non-uniform hydrides distribution. A redistribution of hydrides is related to the high mobility of the hydrogen interstitial atoms at elevated temperature followed by a re-precipitation. Further, the hydrides morphology and orientation with respect to mechanical loading plays an important role for the spent fuel integrity after unloading, for handling, intermediate dry storage and transportation to the final storage facility. The risk assessment based on the hydrogen distribution and quantification along the cladding wall is of high importance for cladding manufacturers, utilities and regulators.

Hydrogen quantification with high spatial resolution, especially in liner cladding, is generally difficult or not possible by common methods like hot gas extraction or metallography. Therefore, high-resolution neutron imaging is becoming an important tool for the hydrogen/hydrides evaluation in combination with microstructural characterization techniques.

High-resolution neutron imaging, using the PSI Neutron Microscope, has become an excellent non-destructive tool providing a hydrogen quantification in un- and irradiated nuclear fuel claddings, with a sub-10 μm resolution and sub-10 wppm sensitivity to hydrogen concentration. In this respect, neutron imaging has allowed unique investigations of hydrogen in highly radioactive fuel cladding sections after service in nuclear power plants.

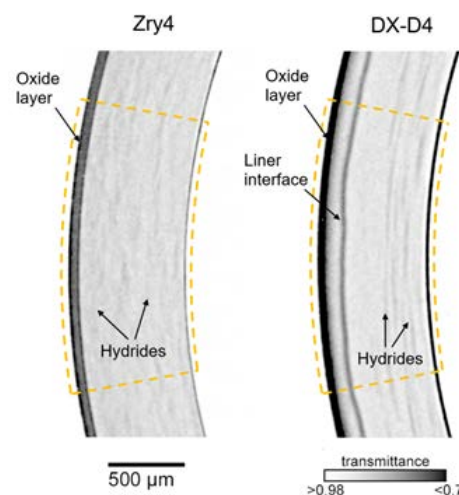


Fig. 1: High-resolution neutron imaging of hydrogen/hydrides in irradiated nuclear fuel cladding.

Development in ATF

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PSI, Laboratory for Reactor Physics and Thermal-Hydraulics, CH-5232 Villigen PSI, Switzerland

ATF –Accident Tolerant Fuels– are alternative material options for fuel and cladding and sometimes control rod that differ slightly (evolutionary) or drastically (revolutionary) from conventional materials. Among other requirements, ATF must exhibit a superior behaviour to the materials used nowadays, under accident conditions particularly (see fig.1).

For several years now, the international industry has received a considerable financial support for the development of ATF. Although Switzerland does not develop any ATF materials, the Swiss NPPs irradiation programmes have been noticeably ahead of the other countries'. The development, modelling and testing of ATF have given place to collaborative activities between different institutions, including the Swiss NPPs and the PSI. In particular, swissnuclear has supported ATF research at PSI with several projects. The presentation relates the history of ATF development and research over the last decades and introduces the current challenges while focusing on the major candidates.



Fig. 1: An exaggeration of a utopian ATF solution

Uncertainty and sensitivity analysis in reactive transport modelling: application to cesium sorption in clay

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Characterization, propagation and analysis of uncertainties are key elements of modelling, especially in presence of complex models involving many, interrelated parameters. Besides informing on the confidence of the results, proper uncertainty analysis identifies the model parameters that drive the result uncertainty, suggesting where to devote data collection efforts. The present work is a result of the collaboration between three research groups at PSI and ETH Zurich, combining probabilistic methods and deterministic models, pioneering the uncertainty and sensitivity analysis of a detailed sorption chemistry model used in Cesium reactive transport modelling, of relevance for geological repository for nuclear waste (Ayoub et al, 2020). From twelve assumed uncertain parameters, the analysis yields major influence of equilibrium sorption reaction constants of Cesium on Type2 and FES sites, in addition to the concentrations of the cations involved in these reactions (Na^+ and K^+) on the diffusion of Cs through clay. Uncertainty in the parameters of the reactive transport model (MCOTAC, Pfingsten, 1994) is analysed combining the Morris method, followed by an extensive Sobol uncertainty analysis (Saltelli et al., 2008). Classification trees are also built to visualize the combination of input parameters' values that could lead to high Cesium concentrations at specific locations. Our findings enable scientists to focus their experiments on important uncertain parameters as well as suggest geometrical setups to increase data collection efficiency.

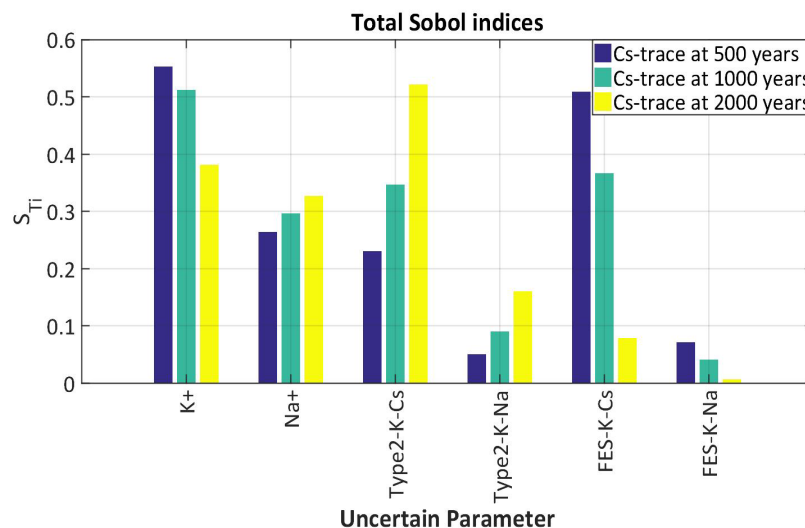


Fig. 1: Parameters driving uncertainty in Cesium transport through clay (Sobol indices, S_{Ti})

References

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- [2] Saltelli et al. (2008). Global sensitivity analysis: the primer. John Wiley & Sons.
- [3] Ayoub, A., Pfingsten, W., Podofillini, L., Sansavini, G. (2020). Uncertainty and sensitivity analysis of the chemistry of cesium sorption in deep geological repositories, Applied Geochemistry, Volume 117, 2020, 104607, ISSN 0883-2927, <https://doi.org/10.1016/j.apgeochem.2020.104607>.

Current status of the GIF Systems and their development in Europe

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The Generation IV International Forum (GIF) is a cooperative international endeavor launched in 2001 to carry out research and development of next generation nuclear energy systems. A set of goals were formulated and six nuclear reactor types were selected for further development. These goals and main features of six reactor types will be briefly introduced in the presentation together with the brief review of recent Euratom projects dedicated to design, safety assessment, R&D and licensing for Generation-IV fast neutron systems.

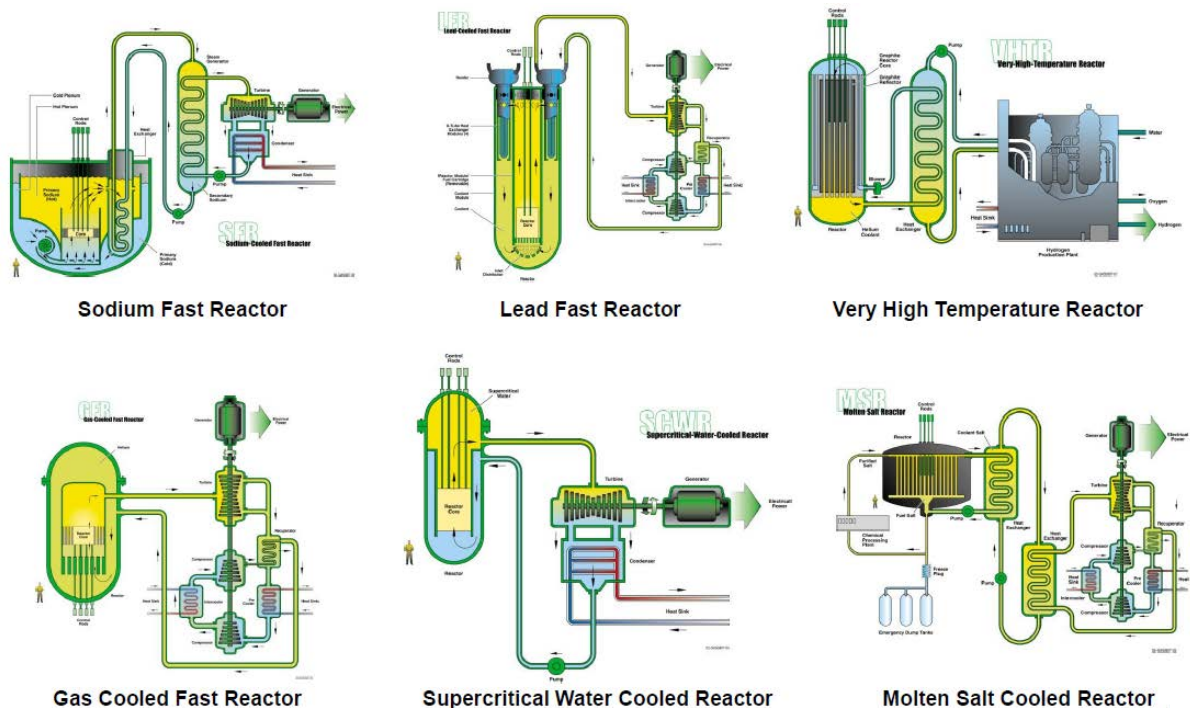


Fig. 1: Main Generation-IV reactor concepts

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Characterization of Strain Localization under Cyclic Loading through Microscopic Digital Image Correlation

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Fatigue damage of materials occurs under cyclic loading due to the heterogeneous distribution of strains at the microstructural scale. In various components of the primary cooling circuits of nuclear power plants, the material experiences multiaxial cyclic loads, which can be proportional, non-proportional, or a combination of both. The effect of different multiaxial cyclic strain paths emerges first at the material microstructure in the distribution of plastic strains, and in turn, this has a significant impact on the macroscopic fatigue damage. To account for microstructural variations and their interactions under relevant loading conditions, macroscopic fatigue responses of the materials are predicted using microstructure-based deformation models. The validation of respective models, however, requires an experimental technique providing information on how strains distribute at the same length scale. Digital Image Correlation (DIC) is a versatile experimental technique, which we use for in-situ, quantitative analysis of local strain distributions at the material microstructure when subjected to complex loading conditions. One of the challenging aspects of performing DIC measurements is the application of speckle patterns on the sample surface suitable to characterize strain fields at the length scale of interest. Because of the limited availability of such a technique, a new patterning approach has been followed using Nanoimprint Lithography (NIL). NIL involves transferring pre-designed pattern templates onto specimen surfaces with the flexibility of scaling the feature details of the DIC pattern to the desired dimensions. Hence, this pattern application technique enables us to conduct high magnification-DIC measurements using an optical imaging system and detect micro-scale strain fields with high precision. In this presentation, the aspects of the DIC measurements using a newly developed patterning methodology will be discussed regarding the investigation of the local deformation behavior of materials under complex loading conditions.

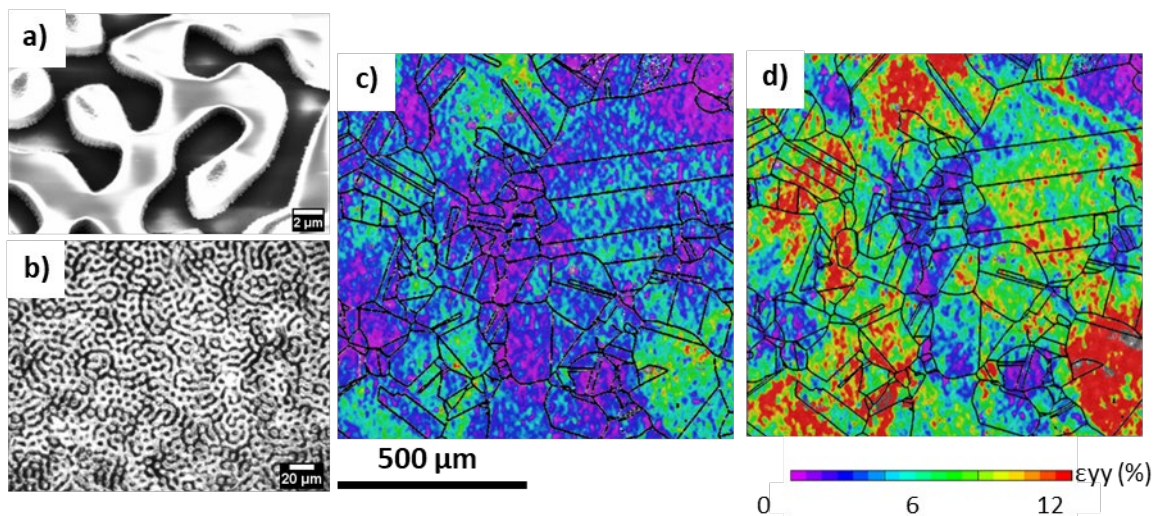


Figure 1: a) Scanning electron microscopy, and b) optical microscopy images of nanoimprinted speckle patterns used to conduct DIC measurement c) and d) DIC contour plots (strain maps) showing grain-scale strain localizations at the different stages of deformation

Development of a crack arrest toughness measurement techniques using small specimens to evaluate the fracture behavior in the ductile-brittle transition region of “ferritic” steel.

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Neutron embrittlement of nuclear reactor vessels made of ferritic steels is one of a key parameter limiting the life of power plants. Owing to the small volume of available irradiation facilities and the limited number of neutron-irradiated surveillance specimens, techniques to measure initiation fracture toughness with small specimens have been developed over the years. Although arrest toughness is of equal importance regarding safety assessment, the emphasis has been put on the effect of specimen size on initiation toughness and practically no small specimen test technique is to be found for arrest toughness measurements. Thus, the objective of the current work was to develop experimental techniques for measuring the initiation and arrest toughness of ferritic steels with miniaturized specimens. Small specimens were produced with a brittle thin layer, which enables crack initiation, was created by surface laser treatment. The cracks were arrested in the more ductile ferritic matrix. The dimension of the specimens was optimized both experimentally and computationally. The test fixture was modified with the guidance of numerical simulation results. Series of successful tests were carried out on tempered martensitic steel (Eurofer97) cantilever beams from -125 °C to room temperature with different types of microstructures. The mechanical tests showed that brittle fracture could be triggered over a temperature range of more than 100 °C for different kinds of specimens and the running cracks arrested occurred in the ductile part of the specimen.

Keywords: Fracture arrest toughness, miniaturized specimens, ductile to brittle transition region, test technique.

H-Uptake (HyUp) – Searching for the causes of increased hydrogen uptake at high burnup in light water reactors (LWR)

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This project concerns research on the causes of increased hydrogen uptake at high burnups in Zr based claddings. Hydrogen ingress into the fuel claddings and its precipitation as hydrides causes changes of chemical and mechanical properties of the cladding. These changes become a safety issue for the cladding in service, and subsequent operations of handling, transportation and dry storage of the spent fuel. It is therefore of interest to minimize the hydrogen content. Understanding the mechanisms of hydrogen uptake and its control, are of high interest. The project has focused on the study of cladding materials from Swiss nuclear power plants.

Hydrogen is created due to the oxidation of the cladding surface. Zirconium has a high affinity to react with hydrogen, and the oxide layer acts as a barrier layer for the ingress of hydrogen into the metal. However, depending on the alloy, this protectiveness is modified with residence time. The microstructure, composition and mechanical properties of the oxide are subject to continuous modification during fuel rod operation, which leads to a changed behavior. The relevant parameters leading to this change are:

- Increased micro-porosity of the oxide layer with increasing burnup. The microstructure of the oxide has been visualized after different numbers of reactor cycles, by subsequent cutting of nanometric slices in a focused ion beam device (FIB), see Fig. 1.
- Changes in the intrinsic mechanical properties of the oxide. The internal stresses have been verified by X-ray diffraction analyses using a micrometric synchrotron beam at the Swiss Light Source (SLS) and by micro-mechanical tests of micro-pillars.
- Change of chemical properties of the oxide layer (inherited from the underlying irradiated metal) leads to variations in the (semi-)conducting properties of the oxide, having influence on how far electrons can diffuse outwards through the oxide, leading to a recombination of H_2 followed by its release. Direct oxide conductivity measurements in an SEM have revealed a decreased oxide conductivity for increased reactor cycles.

Through the project, three PhD theses have been achieved, several students have been guided, and numerous scientific articles have been published. The project has been finalized end of 2020.

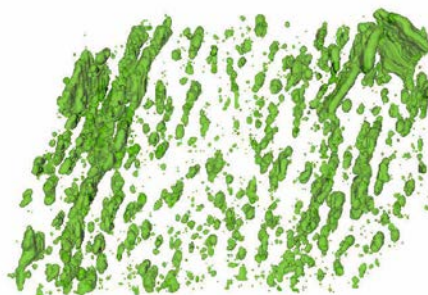
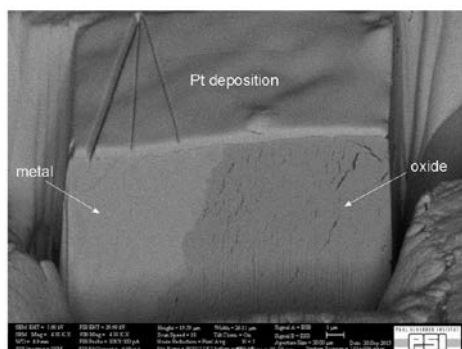


Fig. 1: FIB segment cut into the oxide of the fuel cladding from a 9 cycle rod and 3D reconstruction.

Synchrotron X-ray diffraction and spectroscopy for analysis of crystal defects and fission product speciation in irradiated UO_2 fuels

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Radiation damage effects and fission products behavior in UO_2 nuclear fuel are key issues in understanding and for the modeling of the performance and safety of nuclear fuels in the reactor. In general, the overall performance of standard UO_2 at high burnup is often limited by the phenomena of pellet-cladding interaction, fuel swelling and fission gas release. Therefore, alternative fuel materials with improved properties have been uncovered, such as chromia-doped UO_2 , capable to resist the above listed effects. The present work reports an experimental investigation on irradiation induced microstructure evolution in chromia-doped UO_2 considering the role of dopant Cr and effects of fission

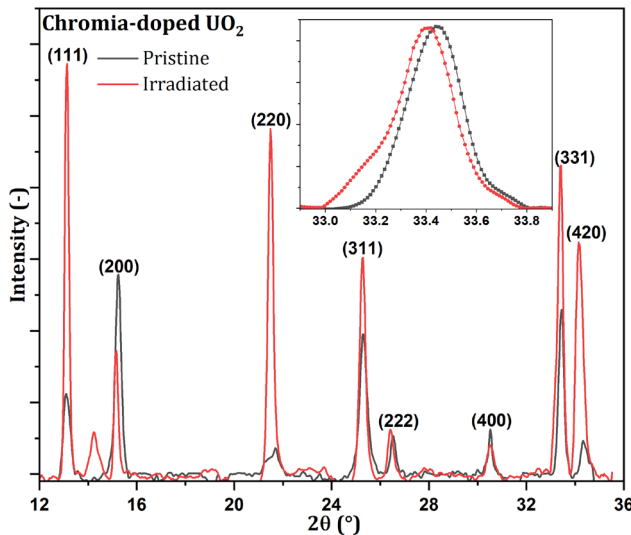


Fig. 1: XRD patterns of unirradiated and irradiated UO_2 . The inset shows enlarged line profiles of the (331) reflection.

product elements, as compared to the standard (i.e., not doped) ones. The materials used for the investigation are industrial grade standard UO_2 and doped UO_2 , both fresh and irradiated fuel pellets. The irradiated pellet, having an average burnup of about 40 MWd kg^{-1} in the pellet, stems from a commercial light water reactor. Synchrotron based analytical methods of micro-beam X-ray diffraction and X-ray absorption spectroscopy (XAS) are used to probe the specimens. Measurements have been made on sub-samples covering a wide range of local burnup from 30 to 70 MWd kg^{-1} in the spent fuels.

Maps of Laue measurements in scanning-mode have been collected in transmission mode by exposing the fuel samples to synchrotron light with 2-seconds exposure time for single-shot images captured. The Laue diffraction images consist of a number of Laue spots. From the spot locations and integrated X-ray diffraction data (Fig. 1), UO_2 lattice parameter, strain in the crystal lattice and deposited elastic strain energy have been determined. For the irradiated fuels, although a number of differences in all Laue images have been noted due to defects accumulated in the UO_2 crystallites, we have particularly examined the local azimuthal rotation in the curved Laue spots patterns. The unpaired dislocation density for each irradiated specimen is determined utilizing the Cahn-Nye analysis and a measured Laue spot streak length. Within the plan and scope of this project, a part of the work concerns XAS investigation of relevant structural phenomena concerning the volatile fission product Sr of nuclear interest. The chemical properties and next neighbor Sr atomic environment have been analyzed considering the limited Sr solubility in UO_2 matrix in addition to the formation of strontium oxide phases as well as other fission-products compounds (such as SrZrO_3) normally found in spent UO_2 nuclear fuels. The results show that majority of Sr is distributed in the chemical form of SrO in the fuel matrix.

HYMEC – HYdrides & MEchanics

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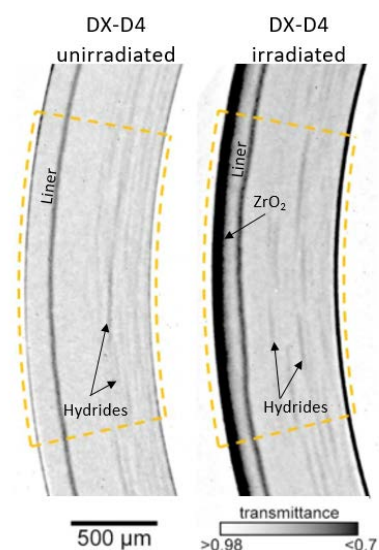
Hydride precipitates in zirconium-based fuel claddings constitute a factor of risk for the integrity of spent nuclear fuel rods, especially during transport and handling necessary before and after intermediate dry storage. The main reason is that hydrides are more brittle than the metal matrix. The pick-up of hydrogen happens due to the waterside corrosion of the zirconium alloy cladding during service in the reactor. Thus, hydrogen is a limiting factor for fuel operation. Diffusion and accumulation of hydrogen in the cladding are driven by the gradients in hydrogen concentration, temperature, mechanical stress and chemical composition. The precipitation into hydrides occurs when the hydrogen solubility limit is reached. It is well known that the mechanical properties of zirconium alloys are directly affected by the presence of these hydrides, for instance, the creep behavior, the fracture toughness and the tendency to brittle failure. Knowledge about the diffusion mechanism, hydrides precipitation and their mechanical influence on the zirconium cladding alloys is important for assessing the failure risk. In this project, the impact of hydrogen on selected cladding materials was evaluated by mechanical testing followed by the characterization of the hydrogen concentration distribution with neutron imaging and SEM/EBSD.

Hydrogen quantification by high-resolution neutron imaging (HR-NI) is an excellent technique that allows quantifying inhomogeneous hydrogen fields at the spatial resolution of $<10\text{ }\mu\text{m}$. Various non-irradiated and irradiated cladding materials, also with a liner, that are currently serving in the Swiss nuclear power plants were evaluated. Quantitative HR-NI studies showed that the hydrogen diffuses to and precipitates at the liner substrate interface regardless of the alloy type.

In addition, C-shape samples are effective to create specific radial and circumferential stress distributions that influence precipitation and orientation of hydrides in the cladding. C-shape samples of Zry-4 and DX-D4 with different hydrogen contents and thermomechanical treatments were characterized by HR-NI. Hydrides reorientation happens predominantly in samples without a liner.

To determine the characteristics of Delayed Hydride Cracking (DHC) under dry storage conditions. HR-NI, SEM and OM investigations have been pursued to determine various properties of DHC in Zircaloy-2 with (LK3/L) and without liner (LK3 and SINQ target material). Properties include the threshold stress intensity factor for DHC under various conditions, diffusion and precipitation kinetics of hydrogen under the effect of a liner and irradiation, crack velocities under various conditions, and phase analysis of DHC-responsible hydrides.

Fig. 1: high-resolution neutron imaging, hydrides accumulation in the liner of a un-/irradiated duplex cladding.



Lasso Monte Carlo for Stochastic Uncertainty Quantification in Nuclear Burn-up Calculations

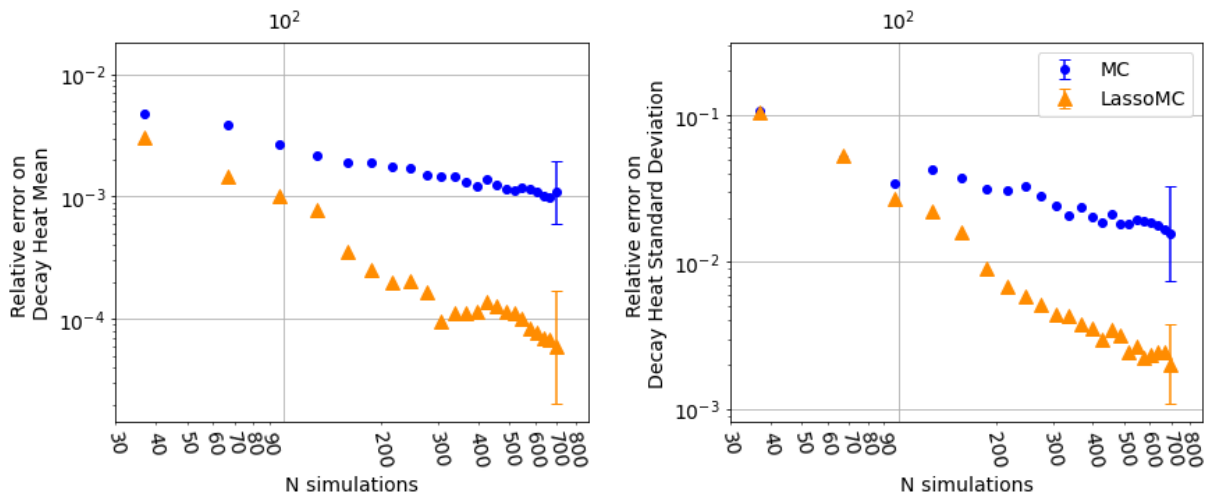
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Nuclear burn-up simulations are used to characterise spent nuclear fuel (SNF). Accurate knowledge of SNF quantities such as decay heat or isotopic composition is necessary to reduce the risks and costs of SNF storage, transport, and disposal, and therefore any uncertainty on these quantities will act as a penalty factor, and needs to be accurately known. It is thus essential that burn-up simulations include uncertainties. Such simulations are computationally expensive and, in order to account for uncertainties in nuclear data, need to be run hundreds of times, a process known as Monte Carlo uncertainty quantification (UQ).

Here we propose a **new variance reduction technique that speeds up UQ**. This method, referred to as Lasso Monte Carlo (**LMC**), combines multilevel Monte Carlo techniques with Lasso regression. The Lasso machine learning technique is able to generate sparse regularised models, that can learn high-dimensional problems such as that of nuclear data UQ, while multilevel Monte Carlo offers a framework to combine models of different fidelities. We show that a **LMC converges 5 to 8 times faster than regular MC** when computing decay heat and isotopic composition of SNF.

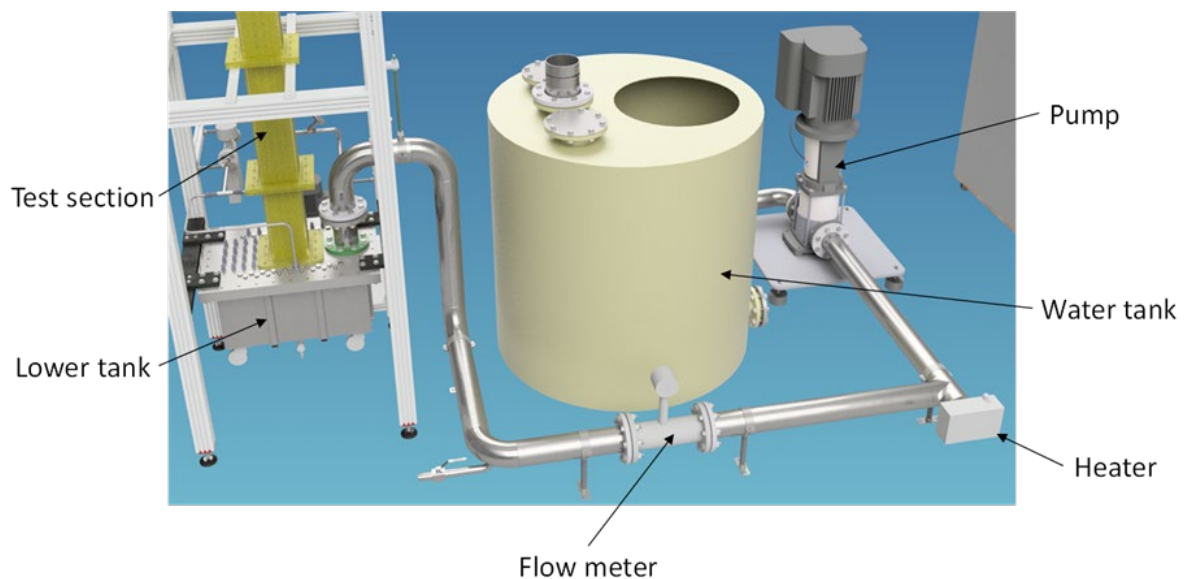


SUBFLOW for Polydisperse Model development (SUPERMO)

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Gas-liquid two-phase flow is a very complex physical phenomenon. It is essential to observe the physical interactions between gas and liquid phases, which can improve the accurate modeling of the interfacial transport terms between the two phases. Thus, the simulation of two-phase flow systems will be enhanced. Two-phase flow behavior is highly influenced by flow conditions and the interaction between the bubbles of different sizes and different velocities. Currently, the prediction of bubble size distribution, bubble velocity and interfacial area concentration remain one of the most challenging tasks in analyzing the transport phenomena and simulating the turbulent bubble flows. Accordingly, several experiments have been conducted in tube bundles such as SUFLOW at PSI. SUBFLOW is one of the very few facilities in the world that use the Wire Mesh Sensors (WMS) to investigate the two-phase flow characteristics in tube bundles. In this project, we have utilized the SUBFLOW test facility to generate new high Reynolds' two-phase flow validation database, which includes void fraction, bubble distribution and bubble velocity measurement in a tube bundle. On the other hand, this project focuses on the WMS post processing techniques. A comparison against previous SUBFLOW experimental data is performed in order to ensure the recommissioning of SUBFLOW facility.



Layout of SUBFLOW facility

Spent Fuel Pin Neutron Emission Measurement with Scintillators (NEWS)

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^aLaboratory for Reactor Physics and Thermal-Hydraulics, PSI

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Neutron emission measurements of spent fuel can give valuable insights into the fuels irradiation history. Since neutron emission measurements can be performed completely non-destructively, it is a prime candidate for routine spent fuel analysis, providing data for code validation. Since neutron emission is dominated by spontaneous fission of minor actinides, such measurements are mainly a test if codes can accurately model the neutron capture events necessary to produce these isotopes. As such it complements more traditional spent fuel measurements focused on fission products. Not only does it make sure the codes well in predicting the (for radioprotection very important) quantity of neutron emission, but also gives a check for the codes which is independent of fission events.

To be able to conduct these measurements , a measurement station for gamma emission in the PSI Hot-Laboratory is adapted to be also able to measure neutrons. Most importantly, a new fast neutron detector is being developed specifically for this application, featuring direct fast neutron detection without moderation for good spacial resolution, high intrinsic efficiency to keep measurement times acceptable, and high gamma blindness necessary for the strong gamma background coming from the spent fuel. A first prototype (see figure 1) has been tested successfully in the Hot-Lab on known spent fuel samples. It demonstrated the capabilities of measuring the absolute neutron emission accurately while achieving a resolution of about 2 cm.



Fig. 1: Picture of the detector tested in the PSI Hot-Laboratory during construction

Advanced source term analysis with MELCOR (ASTAM)

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The aim of the project was to assess the effect of chemical speciation of fission products on the source term. In addition, the uncertainty of the source term assessment due to lack of knowledge of chemical speciation of the fission products and selected other parameters was evaluated.

Three main areas of investigation were carried out:

1. Application of c-GEMS to determine **the effect of fission product speciation on the release** from fuel. The calculations were conducted for the VERDON-1 experiment. With the cGEMS, the experimentally observed effect of gas atmosphere (oxidizing / reducing) on the fission product release was reproduced.

2. **Uncertainty and sensitivity analysis of fission product transport** in Phébus FPT-1 test. This was our first effort in making uncertainty quantification (UQ) in severe accident analysis using MELCOR. The work was started by sensitivity analysis to define the uncertain parameters after which the effect of 15 uncertain parameters on the fission product transport was investigated. Two parameters were shown to have a dominant influence on the aerosol transport in the circuit and concentration in the containment atmosphere.

Uncertainty and sensitivity analysis of **gas phase iodine release from contaminated water**. Chemistry code IMPAIR was coupled with uncertainty tool DAKOTA to determine the potential release of gas phase iodine in Fukushima Daiichi unit 3. Two specific events were analysed, release from the contaminated water in the suppression pool during containment venting, and release from the water in the drywell after about 200 hours.

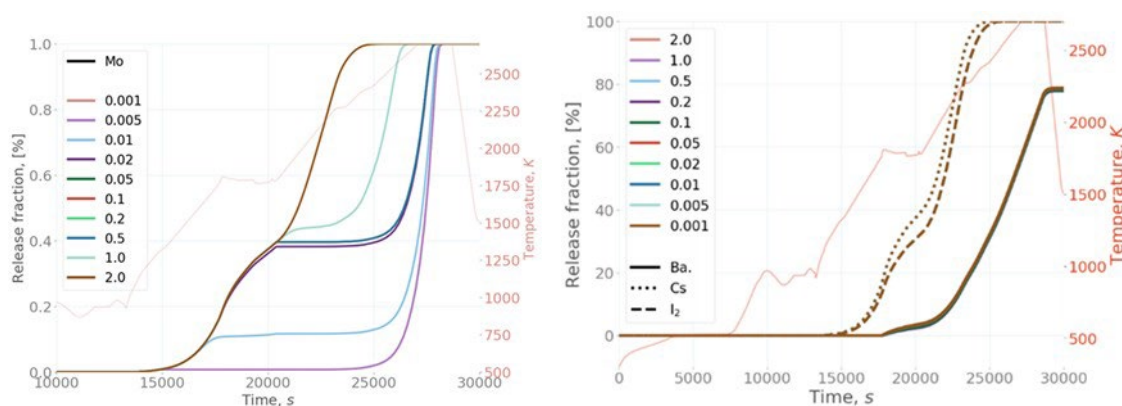


Figure 1. Release of Mo (left) and Ba (right) with different atmosphere scaling factors corresponding to different amounts of oxidizing agent in the gas phase

Hydrodynamic Experiments to Characterize Aerosol Retention (HECTAR)

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One way to mitigate the consequences of fission product releases is to direct the contaminated carrier gas through water pools where a large fraction of the particles may be scrubbed. Current models to predict the particle removal rates in pools are as empirical as uncertain. Computational Fluid Dynamics (CFD) has recently become a mature tool to simulate slow momentum two-phase flows.

The aim of the project is to provide detailed experimental data to enhance hydrodynamics and particle removal models used in pool scrubbing codes. The focus is on two-phase flow bubble hydrodynamics near the injector region, where most of the aerosol mass is removed. The project further aims to validate CFD simulations against collected data with possible model improvements. To achieve that, a series of hydrodynamics and aerosol retention experiments are conducted using the large-scale PSI TRISTAN & ISOLDE and Research Center Jülich (FZJ) SAAB facilities. These facilities are equipped with advanced instruments for multiphase flow and aerosol measurements. The first hydrodynamics tests were performed for low gas flow rates in the range from 0.014 to 0.35 l_n/min and nozzle diameters of 2, 5 and 8 mm. The flow was in the globule regime and was characterized by distinguishable bubbles. The corresponding CFD simulations showed a good agreement in terms of bubble characteristics, i.e. bubble detachment frequency, size, shape and velocity.

However, efficient aerosol retention requires higher gas injection velocities. Accordingly, a test matrix was constructed, in which the gas flow rate ranges from 1 to 10 l_n/min and the nozzle diameters are 5 and 10 mm. These hydrodynamics tests showed that the coalescence and break-up of the globules become stronger. The local averaged void in the injection region reaches the maximum value (void ≈ 1), due to quick succession of the globules creation. The aerosol experiments with the same conditions are foreseen to be conducted in SAAB facility in a collaboration with the FZJ in Germany.

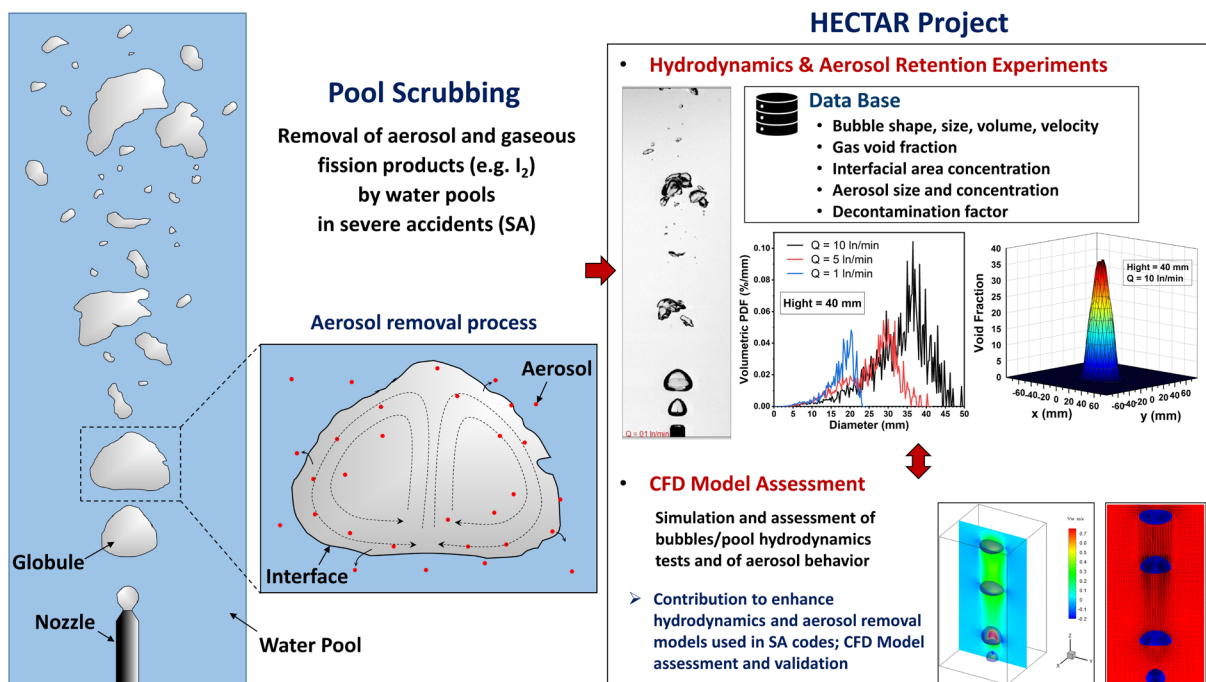


Fig. 1: Bubble hydrodynamics, aerosol behavior and CFD assessment pathway

Numerical prediction of boiling crisis considering surface characteristics

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The goal of the project is to predict the heat transfer and the boiling crisis in fuel assemblies of PWR and BWR by numerical simulations, taking into account wall surface conditions. The outline of the project is illustrated in Fig. 1. First a novel Molecular Dynamics (MD) simulation method has been developed for boiling water in order to predict the contact angle on ZrO_2 with different crystallographic orientations. Second, a new Lattice Boltzmann (LB) method has been developed for multiphase flow with heat and mass transfer, for the purpose to evaluate the influence of surface roughness and contact angle on boiling phenomena. Here, the contact angle computed in MD was used in the LB simulation. The nucleation activation temperature can be predicted as the functions of surface roughness and contact angle by LB simulation, though such a database has not been made yet because 3D simulations were not performed due to heavy computation. The forced convective subcooled boiling flows at the pressure of BWR and PWR have been simulated by using a Computational Fluid Dynamics (CFD) simulation method, yet the computational domain was simple geometry, i.e. rectangular domain. The boiling simulation with locally different wall-surface characteristics has been examined as shown in Fig. 1. The main outcomes of the CFD simulation are the local heat transfer coefficient and the local wall temperature which can indicate the boiling crisis. The boiling model has been implemented to the unstructured CFD code that can take into account the complex geometry in a fuel assembly.

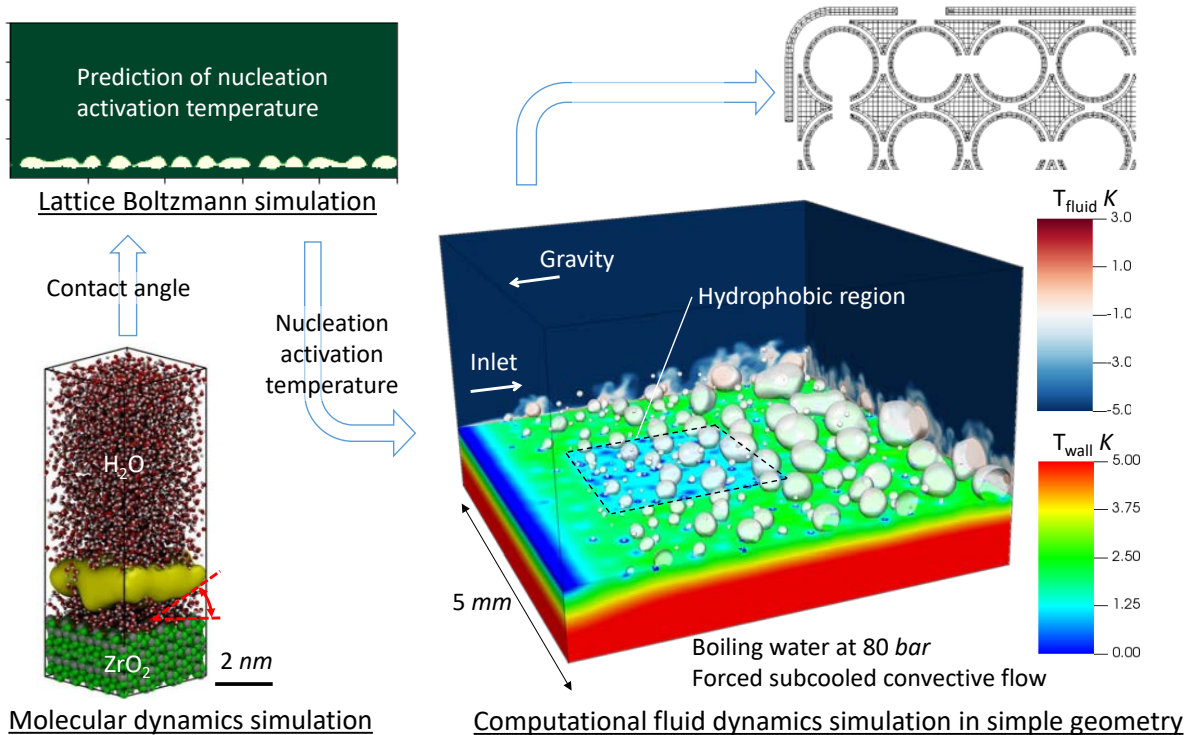


Fig. 1: Numerical simulation of boiling crisis considering surface condition.

ATHESC Thermodynamic modelling of CRUD formation phenomena in LWR

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This project has been focused on improving the understanding of CRUD formation in Light Water Reactors (LWRs) at operation conditions by combining thermodynamic modelling, based on the GEMS code package, with an advanced CRUD characterization.

Significant share of the project time has been dedicated to data collection and an improved calibration of standard thermodynamic properties for the involved mineral substances. The underlying thermodynamic dataset has been validated against the experimental data by computing solubility diagrams at elevated temperatures. For a proper prediction of the inversion phenomena in spinel systems, improved solid solution models have been developed.

Thermodynamic modelling of CRUD formation has been conducted using the improved thermodynamic data and solid solution models. An extensive sensitivity study has been performed to investigate the effects of fluctuations of water composition and temperature on amounts and composition of the precipitates.

The already performed part of the project significantly improves our understanding of CRUD formation phenomena and conditions affecting the precipitation process. A new framework for simulating CRUDs formation using state-of-the-art thermodynamic modeling techniques with the improved thermodynamic database has been established as the main outcome of the project.

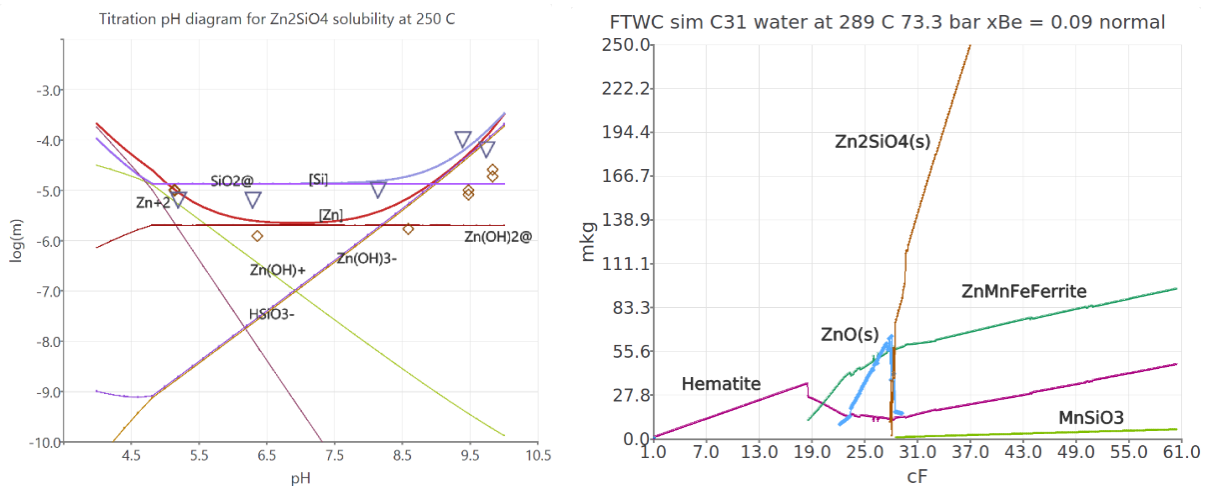


Fig. 1: Solubility pH profiles for willemite Zn₂SiO₄ (left); CRUD deposition at normal oxidizing conditions at 289 °C (right).

MOdelling and CHaracterization of ATF

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Since chromium coating on Zircaloy cladding is expected to reduce corrosion, the reviewing efforts were focused on the oxidation kinetics, in particular in high temperature steam. Several data gaps and limitations have been identified and some safety criteria for Zircaloy should be reviewed for the ATF. A model for high temperature oxidation kinetics of PVD-coated Zircaloy-4 has been developed and implemented in Falcon. A methodology is proposed and applied to a LOCA simulation. Because of the mechanical stresses (boundary conditions) which are not related to oxidation kinetics, both uncoated and coated cladding are expected to burst at a similar time. Concerning oxidation only, the benefits of the coating are clear and the high exposure rod survives the transient while the uncoated one doesn't. The coating may be most beneficial for cladding life extension or for SB-LOCA conditions. Thermodynamic equilibrium modelling has demonstrated an exceptional stability of the Cr_2O_3 compound in KKL operating conditions. As far as severe accidents are concerned, the main improvement in MELCOR with respect to ATF is the inclusion of FeCrAl as a materials group as well as four user defined core materials.

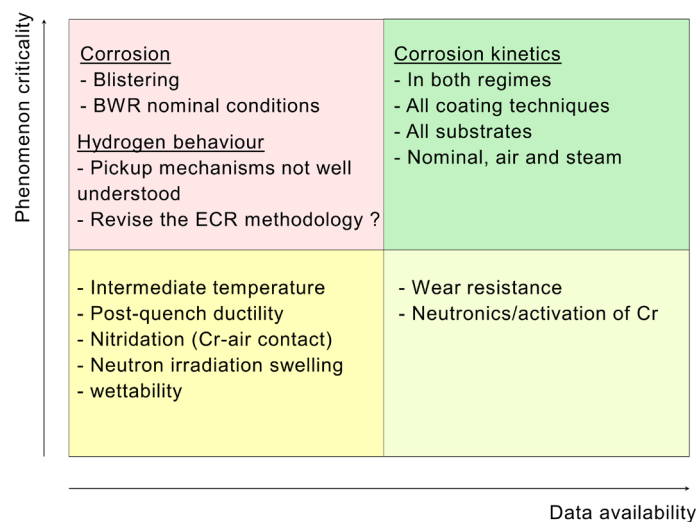


Fig. 1: Status-quo of Cr-coated zircaloy-based claddings