NuFuel-MMSNF 2019 Workshop

Monday 4 November 2019 - Thursday 7 November 2019

PSI Auditorium

Book of Abstracts

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Session 1 / **40**

Development and Implementation of a Thermochemical Database, MSTDB, for Simulating Fuel Behavior in Molten Salt Reactors

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Molten salt reactors (MSRs), with salt as the fuel/coolant or solely the coolant, require a close understanding of salt properties to be able to simulate normal and off-normal operations. Among the most important are the thermochemical properties of the salt, that is the Gibbs energy relations for the complex liquid and solid solutions as these provide thermal properties as well as critical phase equilibria such as solidus and liquidus. Models for the pseudo-binary and -ternary fluoride and chloride salt systems are being compiled, and where necessary developed, to provide a thermochemical resource. The molten salt thermochemical database (*MSTDB*) is being implemented with the thermochemical solver THERMOCHIMICA in prospective MSR codes for use in reactor design, simulating reactor operations, and assessing of off-normal scenarios to support regulatory activities.

The *MSTDB* is a collection of thermochemical descriptions involving existing data in addition to those found through first principles methodologies and experimental measurements. Density functional theory and related methods are being used to obtain solid salt phase stabilities, along with efforts to extend the approaches to the molten salts. Measurements include determining phase equilibria including melting points, crystalline phase structures, and heat capacities, among other properties. This information together with available reported data are being used in thermochemical assessments to obtain consistent and accurate models and values for Gibbs energy relationships in complex, multi-component salt systems provided to *MSTDB*. The thermochemical database is publicly accessible via an on-line code-sharing protocol. In this presentation, a description of the development and state of the database will be provided along with examples of system assessments and demonstrations of applications of resulting equilibrium calculations within developing MSR codes.

This work was supported by the U. S. Department of Energy Nuclear Technology Research & Development - Molten Salt Reactors Program under ORNL/UT-Battelle subcontract 4000160938.

Session 1 / **22**

Thermodynamic, Transport, and Structural Study of the LiF-UF4 System

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The Molten Salt Reactor is a class of innovative nuclear reactor in which the fuel is dissolved in a liquid fluoride or chloride bath. The reference fuel under consideration in Europe for the MSFR (Molten Salt Fast Reactor) is a fluoride salt of composition 7LiF-ThF4-233UF4 (77.5-20.0-2.5 mol%) or 7LiF-ThF4-enrUF4-(Pu-MA)F3 (77.5-6.6-12.3-3.6 mol%) [1]. Despite the giant leaps MSR technology has seen since its conception, there remain important technical issues for the technology to reach commercial maturity. The chemical complexity of the fuel salt is one of them. The salt bath is a multi-component system, quite difficult to characterize. It is hence essential for the safety assessment of the reactor to develop models and simulation tools able to predict the physico-chemical properties of the fuel over a wide range of temperatures, compositions and redox potential.
A fundamental understanding of the relationship between the local structure of the molten salt and its physico-chemical and thermodynamic properties is needed to develop such models and gain greater predictive capability over this dynamic, far from ideal salt. It is known that depending on conditions of composition and temperature, the local structure can vary widely with cases where the ions in the melt are completely dissociated, form molecular species, or even exhibit some degree of polymerization [2], [3]. What kind of regime could we expect, say, in different sections of a MSFR? To build a comprehensive model of the multi-component fuel physico-chemical properties requires to perform measurements of simpler sub-systems, from which models can be extrapolated. In order to gain in accuracy, these models should also take into account as much physical information as possible. The approach in this work is therefore multi-disciplinary and includes experimental measurements of physico-chemical properties and local structure, as well as thermodynamic modelling assessments and molecular dynamics simulations. We investigate the link between short-range order and thermodynamic and transport properties in the key system LiF-UF4 and report a comprehensive thermodynamic model based on the CALPHAD method and the quasi-chemical formalism in the quadruplet approximation. We integrate in this model experimental information from (i) in-situ high temperature Extended X-ray Absorption Fine Structure spectroscopy (EXAFS) measurements using a set-up recently developed at the Delft University of Technology (TU Delft, The Netherlands) [4], (ii) phase diagram equilibria and (iii) mixing enthalpy measurements, together with the output of molecular dynamics simulations based on the Polarizable Ion Model (PIM) [5].

Session 1 / **12**

Recent Development of Thermochimica for Simulations of Nuclear Materials

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The open-source equilibrium thermochemistry library Thermochimica has previously been employed to study uranium dioxide nuclear fuel for light-water reactor applications. Recently, significant improvements to the efficiency and range of applications of Thermochimica have been made. We will discuss these advances and demonstrate applications of Thermochimica for next-generation nuclear technologies, such as Molten Salt Reactors (MSRs) and Tristructural-isotropic (TRISO) fuels. Calculations on popular molten salt fuel materials, such as FliNaK, FliBe and fission product containing salts, have been enabled through the implementation of the quadruplet approximation to the modified quasichemical model in Thermochimica, which takes into account first and second-nearest-neighbor short-range ordering contributions to the Gibbs energies of liquid solution phases. Coupling of Thermochimica to various other software packages, such as the Multiphysics Object Oriented Simulation Environment (MOOSE), Coolant-Boiling in Rod Arrays - Two Fluids(CTF), Virtual Environment for Reactor Applications (VERA), and Oak Ridge Isotope GENeration (ORIGEN) for nuclear fuel applications will also be demonstrated.

Session 1 / **103**

GEMS / MELCOR coupling and its application to fission product release simulations

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In recent years, the efforts of the scientific community in developing reliable methods of severe reactor accident analysis have been growing. In this context, the MELCOR code is used at PSI to assess the progression of severe accidents in light water reactor nuclear power plants, including fission product behavior and release to the environment. However, the representation of chemistry in MELCOR is rather limited: the thermodynamic stability of nuclear fuel, as well as reactions of fission products with each other or with structural materials, are not well accounted for. Chemical speciation is limited to a pre-set table of compounds. Meanwhile, PSI has developed a state-of-the-art expertise in advanced chemical thermodynamic modelling of nuclear fuel systems, using in-house Gibbs Energy Minimization (GEMS) codes and a dedicated thermodynamic database (HERACLES) for nuclear fuels with associated materials and gases.
In this work we have focused on combining MELCOR simulations and GEMS chemical thermodynamic computations to deepen the understanding of reactor chemistry and severe accident scenarios. As the first steps of the research the coupled GEMS /MELCOR was used to investigate the vaporization of salt and fission product species from the MSR fuel in accident conditions. Vaporization model of the fuel salt was added to MELCOR and was supplied with the vapor pressures calculated with GEMS. This allowed us to model species retention by the salt mixture compared to the pure compound calculation. Additionally, speciation of iodine, which is effected by the salt composition has been analysed.
Besides, the coupled GEMS /MELCOR was employed to study the FP release from the spend fuel by modelling VERDON experiments. The obtained results allow for more accurate speciation study as well as release behaviour.

Session 2 / **50**

Analysis of fuel rod behavior during design basis accidents using the Bison code

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The US Department of Energy (DOE) has been developing state-of-the-art capabilities to simulate nuclear fuel behavior within the Consortium for Advanced Simulation of Light Water Reactors (CASL) and Nuclear Energy Advanced Modeling and Simulation (NEAMS) programs. The result is the Bison code [1], a modern multidimensional, finite-element based fuel performance code developed at Idaho National Laboratory (INL). Validation work for Bison has focused initially on Light Water Reactor (LWR) fuel during normal operating conditions and power ramps [2]. More recently, significant progress has been made on Bison development and validation for the analysis of accident scenarios such as Loss-of-Coolant Accidents (LOCA) [3,4] and Reactivity-Initiated Accidents (RIA) [5,6].

In this contribution, a brief overview of relevant Bison capabilities is provided, followed by presentation of code results for the simulation of LOCA and RIA experiments. LOCA simulations comprise

separate effects tests of cladding ballooning and burst, and Halden integral fuel rod tests from the IFA-650 series. Comparisons to experimental data include cladding burst pressure and temperature in separate effects tests, as well as the evolution of fuel rod inner pressure during ballooning and time to cladding burst in integral tests. Furthermore, Bison three-dimensional simulations of separate effects tests are performed, which demonstrate the capability to reproduce the effect of azimuthal temperature variations in the cladding. RIA simulations include selected power pulse tests from the CABRI and NSRR campaigns, with experimental comparisons focusing on fission gas release and cladding displacement.

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Session 2 / **37**

A burn-up module for application in fuel performance codes: methodology, verification and assessment for MOX fuel in thermal and fast neutron spectra

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The evolution of actinides within the nuclear fuel affects the power distribution and the thermal and mechanical material properties. In addition, the concomitant production of helium in the fuel matrix due to actinide alpha decays and nuclear reactions has a relevant impact on the whole fuel rod performance, since helium concurs to fuel gaseous swelling and gas release. For this reason, fuel performance codes (FPCs) need to incorporate predictive burn-up modules to account for the evolution of actinides under irradiation. State-of-the-art softwares dedicated to depletion calculation (e.g., SCALE, MONTEBURNS, SERPENT) require considerable computational time compared to FPCs, hindering their engineering application in fuel performance simulations. In this work, we propose a new burn-up module for application in FPCs. The burn-up module relies on average microscopic cross-section lookup tables generated via SERPENT high-fidelity calculations, and involves the solution of the (non) linear system of Bateman's equations for a selected subset of relevant actinides. We implemented the model in the SCIANTIX code, a 0D stand-alone fuel behavior code designed for the coupling with FPCs, effectively paving the way for the inclusion of the burn-up model in FPCs. We verified the results of the burn-up module in terms evolution of actinides and helium concentrations for MOX fuel (both thermal and fast reactor conditions) by comparing them with the high-fidelity results from SERPENT. Moreover, for assessment sake, we benchmarked the results of the new burn-up module with those of TUBRNP, the burn-up module currently used in the TRANSURANUS code. The methodology proposed in this work for the development and verification of a burn-up module, which we consider as one of the main outcomes of the work itself, is general and can be adopted for the analysis of any reactor/fuel combination.

Session 2 / **33**

PLEIADES ALCYONE 3.5D simulation of a power ramp including

OpenCalphad fuel thermochemistry with TAF-ID

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ALCYONE 2.1 fuel performance code, co-developed by CEA, EDF and Framatome within the PLEIADES software environment, provides a multidimensional modeling for detailed analysis of PWR fuel elements behavior under irradiation [1]. ALCYONE is validated by comparing numerical results to post-irradiation examinations from a large experimental database. Iodine-Stress Corrosion Cracking is one of the physical phenomena of interest for cladding design and safety analysis in PWRs. Its understanding and its description require knowledge of the fuel thermo-chemical behavior and of the distribution of volatile species such as, iodine, cesium, tellurium and inert fission gas, in the pellet fragment. In order to be able to simulate Iodine-Stress Corrosion Cracking, a significant work has been done since the early 2010s to integrate an accurate thermochemical modelling of irradiated fuel in the PLEIADES platform [2]. Recently, the modelling has been upgraded with the integration of OpenCalphad thermo-chemical solver [3] in order to use the thermodynamics data coming from the TAF-ID, the international project aiming at making a quality-assured database for nuclear fuels. In 2018, first results were presented that show the capacity and robustness of the ALCYONE/OpenCalphad coupling to simulate efficiently complex in-reactor power ramps with the TAF-ID [4]. Since then, the code has also been upgraded to couple the thermochemical modelling with oxygen transport taking into account thermodiffusion [5]. The present study follows from these works. We focus our presentation on 3.5D ALCYONE simulation of a power ramp including OpenCalphad fuel thermochemistry with the TAF-ID. First, the chemical state of fission products calculated during the transient is analyzed and compared to the one obtained with thermodynamics data coming from the TBASE database but also to measurements. Then, a particular attention is paid to the oxygen-to-metal ratio and to the oxygen potential of the fuel calculated with the TAF-ID. The values of these thermodynamics data calculated for several thermodynamics conditions during the power ramp are discussed and assessed against data available in literature. Finally, as a first step towards an improvement of the modeling of oxygen transport in ALCYONE [5], we present calculations of the concentration in vacancies and oxygen interstitials in the different phases considered in the TAF-ID.

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Session 2 / **20**

Multi-scale nuclear fuel simulation with VER software

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PLEIADES is a scientific code platform dedicated to nuclear fuel behaviour simulation for several types of reactors: water cooled

reactors, sodium cooled fast reactors, research and material testing reactors, etc. In this platform, the microstructures of these different types of fuel are studied using VER software (Representative Elementary Volume). These studies aim at the comprehension of the thermo-mechanical phenomena at the microscopic scale, and their homogenisation for implementation of their effective behaviour in fuel performance codes. Here are some applications:

- UO_2 fuel is a poly-crystalline ceramic (Figure 1). The mechanical behaviour of each crystal can be modelled with crystalline plasticity, based on dislocation mouvement. An overall behaviour is then deduced by homogenisation.
- MOX fuel contains heterogeneity due to the variation of Pu concentration on a microscopic scale. This can lead to stress and strain concentration near the Pu rich agglomerate. This heterogeneity can be simulated either with discontinuous geometry (Pu rich inclusions in Pu poor matrix, Figure 2), or with continuous Pu field (Figure 3). The macroscopic mechanical behaviour is established using homogenisation methods such as Mori-Tanaka or reduction techniques like Nonuniform Transformation Field Analysis.
- In some fuels, flat porosity is formed around the agglomerates. Simulations of these microstructures are carried out (Figure 4) in order to study the degradation of the fuel conductivity due to this porosity.
- For accident tolerant fuel, new concepts are studied, such as adding a highly conductive phase to the fuel. This is shown in Figure 5, where the metal phase around the agglomerates enhances the pellet conductivity.

Session 3 / **18**

New helium equation of state for pressurized nanobubbles in UO2 matrix calculated via molecular dynamics simulations

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During storage helium atoms accumulate in spent fuel via alpha-decay. These helium atoms cluster into microscopic bubbles that change the physical properties of spent fuel. To estimate the impact of such bubble, it is essential to possess a good thermodynamical model for helium interacting with the surrounding matrix including states at high pressures and temperatures.
Therefore, molecular dynamics simulations are carried out to establish a new equation of state for helium in nanobubbles embedded in UO2 matrix. Four bubbles sizes, ranging from 1 to 10 nm, have been investigated for temperatures ranging from 300 to 900 K and helium concentration ranging from 3.2×10-2 to 0.39 mol/cm3. From these data, we are able to fit a new equation of state for helium using the Brearley and MacInnes'model.
We observe that helium atom is heterogeneously distributed inside the nanobubble with the apparition of a boundary layer of about 1 nm thick at the surface. We also find an upper limit concentration corresponding to 1.6 helium atom per UO2 vacancy beyond which no more helium atom can be incorporated into the bubble.

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2-D and 3-D modelling of fission gas release due to intra-granular bubble movement during post-irradiation annealing of UO2 fuel

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High values of fission gas release from UO_2 fuel during post-irradiation annealing tests cannot be explained by the effective diffusion theory, which is generally used in the modelling of base-irradiation of nuclear fuel. Since the fission gas atoms are highly insoluble in the bulk UO_2, they mostly precipitate as intra-granular bubbles. Movement of these highly pressurized intra-granular bubbles has been proposed as one of the mechanisms of fission gas release. The difficulty in modelling the movement of intra-granular bubbles is that these bubbles are extremely small (~ few nm) and numerous while the grain radius is about 5µm. To tackle this problem, a new spatialized mesoscale model was developed where individual bubbles are described, along with the diffusion of vacancies from each bubble to the other, as well as from the free surface. Using this model, two scenarios, and the combination of those, have been assessed for the fission gas release. First is the movement of bubbles in a vacancy gradient, and second is the random movement of bubbles. The analyses have shown that neither of these two scenarios, nor the combination of them, could explain the large fission gas release obtained during post-irradiation annealing in our reference experiment.

A third scenario was also tested, in 3-D but on a smaller domain, by considering the pinning of intra-granular bubbles on dislocations and their movement along with the dislocations, via the mechanism of 'dislocation climb'. The dislocation climb mechanism has been demonstrated as a prominent gas release mechanism scenario, however, the values for diffusion of vacancies on the dislocations are not known. The results obtained help us to distinguish the fission gas release scenarios that could really explain the observations during post-irradiation annealing tests.

Session 3 / 21

Design of a novel set-up for the investigation of helium behaviour in oxide nuclear fuel via infusion: realization, modelling and preliminary results

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In this work, we present a newly designed experimental set-up to infuse helium in UO2 samples. The objective of the presented activity is to carry out experiments aimed at investigating helium behaviour in nuclear fuel, measuring its key properties such as diffusivity and solubility. The proposed experimental set-up consists of a laser-heated autoclave (continuous-wave 4.5 kW Nd:YAG laser at 1064 nm) that can operate at pressures up to 400 MPa. The high temperature that can be achieved combined with the effect of the high pressure allow a very fast saturation of the sample, up to the helium solubility limit, in only a few hours. The laser beam passing through a sapphire window placed on the upper part of the autoclave hits the sample and heats it up to around 850℃, temperature that ensures the achievement of the helium solubility limit but minimizes the risk of grain growth. In fact, the main feature of the samples used in this experiment consists in their grain

size. The samples are disks of sintered UO2 characterized by nanometric grain size (down to about 100-50 nm) used in order to assess the effect of the presence of numerous grain boundaries. This aspect becomes technologically relevant if one considers the microstructure of nuclear fuel irradiated at current discharge burnups where the so-called high burnup structure (HBS) is formed. Moreover, the laser spot size exceeds that of the sample and in order to reduce temperature gradients between the sample and the crucible we have designed and manufactured a custom sample holder made of the same material as the sample itself. The tailored sample holder consists of a zirconia piece, acting as a thermal barrier, topped by a UO2 disk with a central recess in which the UO2 sample is positioned. In addition, the temperature is measured by an infrared pyrometer facing the sample surface and aligned along the same optical axis as the laser beam. After the infusion, we measured quantitatively the helium release from the UO2 sample in a Laser Knudsen Cell (LKC) by means of the Quantitative Gas Measurements System (Q-GAMES) developed at the JRC.
Lastly, the experimental results obtained have been used for a preliminary validation of a new physics-based model developed for describing the helium behaviour in oxide nuclear fuel, accounting for its production, solubility and diffusivity. The verification and validation of this new comprehensive model have been performed in SCIANTIX that is a stand-alone code developed at POLIMI for the simulation of separate-effect test experiments, and will be used to improve fuel performance codes such as TRANSURANUS.

Session 3 / **34**

Noble gas transport in UO2 annealed under controlled O2 partial pressure: first results

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In collaboration with CEMHTI/CNRS Orléans, DEC/LLCC/CEA Cadarache, JRC-Karlsruhe and in the frame of INSPYRE WP 2.2, we study the behavior of noble gases (Kr, Xe) in UO2 using Thermo-Desorption Spectrometry (TDS). The presented work is a continuation of a separate effect studies where numerous parameters have already been evaluated: the nature of the implanted ions, their energies, their fluence, irradiation defect concentration, UO2 microstructure and its preparation, etc. It notably made possible to experimentally demonstrate that the transport of noble gases are greatly influenced by the presence of traps that will efficiently retain the noble gases in the fuel. The partial pressure of oxygen is another fundamental parameter which we were up until recently unable to impose and vary during TDS experiments. It is however of prime importance since stoichiometry is already known to strongly influence noble gases diffusion kinetics and mechanisms in UO2±x.
On our PIAGARA platform, we recently implemented a laser heating line specific to nuclear materials. This system is coupled to a gas purification line and a high sensitivity noble gas mass spectrometer that allows studying annealings under optimal environmental conditions (pseudo-levitation) and a large range of temperatures (600-2500°C). For oxygen studies, we have included an oxygen sensor and an O2 trap that allows us to control the partial pressure of oxygen (pO2) prevailing in our heating system. The LLCC provided us with a panel of samples manufactured under controlled pO2 and then packaged under vacuum or air. We will present the first results of these experiments and we hope to show the effectiveness of our O2 control system. We will also compare these controlled pO2 experiments with our previous ultra-vacuum TDS data.

Session 4 / **51**

Steam oxidation of SiC at high temperatures studied by laser heating method

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Silicon carbide (SiC) has recently attracted much attention as a potential material for accident tolerant fuel cladding. To investigate the performance of SiC in severe accident conditions, study of steam oxidation at high temperatures is necessary. However, the study focusing on steam oxidation of SiC at temperatures above 1600ºC is still certainly limited due to lack of test facilities. With the extreme oxidation/corrosion environment in steam at high temperatures, conventional refractory materials, i.e., alumina, zirconia, W, Mo and so on, would not survive during the tests. Application of laser heating technique could be a great solution for this problem. Using a laser heating technique, we can localize the heat transfer and focus them on the test sample only. This paper presented the outline of the laser heating facility and recent results on high-temperature oxidation of SiC in steam in temperature range between 1400 and 1800ºC (for 1-7 h). The oxidation kinetics is then discussed based on the weight gain and observation on the cross-sectioned surface of tested samples. Mechanism of bubbling observed in our samples above approximately 1750 ºC is also discussed.

Session 4 / **30**

Thermochemical Modeling In-Reactor Behavior of Uranium Silicide-Based Accident Tolerant Fuels

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Uranium silicide fuels have been proposed as part of accident tolerant fuel concepts for light water reactors. Uranium silicides (U₃Si₂ and U₃Si₅) have increased uranium atom density over UO₂ fuel and thus their use can offset neutronic losses from more robust replacements for current zirconium-based cladding. Further development of such fuels, however, requires a thorough understanding of their thermophysical and thermochemical properties under reactor conditions. Interactions between the fuel and cladding materials and fission products produced during burnup are also necessary to consider in order to fully evaluate any fuel candidates. In the current work, a combination of experimental and computational methods was used to model these accident tolerant fuel candidates to generate a thermochemical database for implementation in fuel performance codes.

The U-Si binary within the 40-66 at% Si region was explored to understand and model compositional changes that may occur during reactor operation. Samples of varying compositions were produced using arc-melting and characterized through electron microscopy, neutron and x-ray diffraction (XRD), and differential scanning calorimetry (DSC). First principles modelling was used to supplement experimental results and the CALPHAD method was used to assess U-Si and calculate phase equilibria. To consider the impact of more robust cladding materials on accident tolerance

of the fuel, the compatibility of U₃Si₂ with FeCrAl and SiC/SiC composite claddings was investigated and compared with a baseline study of U₃Si₂ and Zircaloy-4 compatibility. High temperature diffusion couples of fuel and cladding were used to simulate over-temperature or extended burnup in-reactor behavior and electron microscopy and XRD were used to characterize the fuel/cladding couples. DFT and CALPHAD calculations were used to aide in the interpretation of experimental observations.

The interactions of silicide fuel and fission products resulting from burnup were simulated using U₃Si₂ doped with up to five surrogate fission products (Ce, Gd, Mo, Y, Zr) and the production of a "SIMFUEL"representative of high fuel burnup. Structural changes and secondary phase formation from heat-treated samples was characterized using microanalytical techniques, neutron diffraction, and XRD. The impacts of more volatile fission product species were considered using DFT and a CALPHAD database was developed.

Session 4 / **47**

Fuel Thermomechanical modelling with Falcon at PSI

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The EPRI code FALCON MOD01 has been used at PSI for about two decades for both research purposes and safety analyses, and is still undergoing developments. Namely, its coupling to the advanced fission gas release and swelling module (GRSW-A) module allowed the developments of several methodologies such as void formation by high temperature restructuring and burst fission gas release in RIA conditions. Besides, PSI is co-developer of the newer version of the code Falcon V1. In this respect, the FALCON MOD01 developments can be transferred to the newer version. In addition, other aspects are directly treated such as H-uptake or implementation of behavioral models for several ATF concepts in order to assess their performance.

Poster flash talks / **6**

Finite element modeling of fuel behavior based on the MOOSE framework

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Abstract: Fuel performance modeling and analysis plays an important role in fuel design and performance optimization, especially accurate fuel rod modeling and analysis in 3D. Fuel thermal behaviors are very complex and are strongly coupled with other factors. For example, with the increase of burnup, fuel thermal conductivity decreases which further increases the pellet central temperature, and gap distance becomes smaller during the swelling of the pellet, because of the accumulation of solid fission products, fission gas and pellet thermal expansion which decrease the pellet central temperature in turn. So fuel performance modeling is inherently a multiphysics problem. In this paper, we established a 1/4 pellet-cladding model containing modules for heat transfer, mechanical analysis, and fission gas release calculation, etc, based on the MOOSE finite-element framework. This paper demonstrates our current experiences in applying the MOOSE framework to PWR fuel behaviors simulations.

Poster flash talks / **7**

Microstructural evolution of Fe-9Cr alloys under 3.5 MeV Fe13+ ion irradiation

Authors: Tiantian Shi[None]; Di Yun[None]

Abstract: The microstructural evolution of two Fe-9Cr model alloys with different C content after irradiation was investigated by transmission electron microscopy. These two steels were both irradiated with 3.5 MeV Fe13+ ions at 450℃ to a peak damage level of 3 dpas. TEM results indicate that <100> loops and 1/2<111> loops coexist in the two irradiated steels. Furthermore, the loop size of Fe-9Cr alloy with higher C content is about twice that of the Fe-9Cr alloy with lower C content. The difference in the size of the dislocation loops between the two steels may be attributed to the difference in C content. The carbon–vacancy complexes are effective traps for SIA loops and contribute to the growth of the loops, which may cause larger size dislocation loops in Fe-9Cr alloy containing higher C content.

Poster flash talks / **8**

Atomic scale modelling of stoichiometry deviation in amorphous zirconia

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A combination of materials modelling techniques and targeted experimental investigations have identified the manner in which non-stoichiometry is accommodated in both crystalline and amorphous ZrO_2. Not only is excess oxygen possible in both crystalline and amorphous ZrO_2, but it is found that there is a high propensity for significant deviations–especially in the amorphous system–forming ZrO_{2+x}. This has clear implications to the behaviour and degradation of ZrO_2 as the boundary oxide protecting zirconium alloys within a water cooled nuclear power reactor.

Poster flash talks / **13**

Release of volatile fission products (Xe, Kr, I, Cs) implanted in polycrystalline UO2

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Under irradiation in nuclear reactors, the microstructure of oxide nuclear fuel changes. To improve the modeling of the UO2 fuel behavior under irradiation, it is necessary to understand the elementary mechanisms of fission products diffusion. Among them, rare gas Xenon and Krypton represent 30% of created elements moreover fission products such as Iodine and Caesium are corrosive for the

clad. Our experimental work consists in the measurement of the release kinetics of stable isotopes of these fission products by Knudsen Cell Mass Spectrometry. In that aim, 8mm diameter-1 mm height fresh polycrystalline UO2 pellets are implanted with different concentrations in 129Xe, 83Kr, 127I, 133Cs to understand the effect of the fission products density on the diffusion. The release kinetics is studied either during the heating at a given heating rate from room temperature up to about 1400℃ or during isothermal annealing.

At the same time, we are trying to model the mass spectrometer signal obtained to deduce information about the fission gas and products transport.

Poster flash talks / **15**

Experimental study of Joint-Oxyde-Gaine (JOG) systems in Fast Neutron Reactors

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Advanced Generation-IV nuclear reactors, which should excel in the areas of sustainability, economics, safety & reliability and proliferation resistance, are currently being developed to replace the Light Water Reactors (LWRs) at the end of their operating licenses. Among the various designs selected by the Generation-IV International Forum, research has been focused in Europe on fast neutron reactors cooled by Sodium (SFRs) or Lead (LFRs). (U,Pu)O2-x mixed oxide is currently the reference fuel for these reactors. Considering the higher temperatures, thermal gradients and neutron flux of SFRs and LFRs in comparison to LWRs, the behavior of the fuel can be significantly different. The European INSPYRE (Investigations Supporting MOX Fuel Licensing in ESNII Prototype Reactors) project of the 2016-2017 Euratom H2020 Fission call has started in 2017 with the investigation of the (U,Pu)O2 fuel behaviour under irradiation to support the licensing of next generation SFRs and LFRs [1]. One of the several objectives of this project is to model the formation of the so-called JOG layer (Joint Oxide Gaine), that forms between the fuel and the cladding following the migration of volatile fission products, such as Cs-Mo-Te-I, from the inner pellet towards the outer rim [2]. In this context, this work aims to obtain reliable experimental data for this multi-element system and use them to develop thermodynamic models based on the CALPHAD methodology.
Our progress on the experimental investigations of the JOG sub-systems will be presented at the NuFuel conference. In particular, our most recent results on the Cs-Mo-O, Cs-U-O, Ce-Te-O, and Cs-(Te,Mo)-O systems will be reported: structural characterizations using XRD and neutron diffraction, determination of enthalpies of formation by solution calorimetry, melting/transition temperatures and melting/transition enthalpies by Differential Scanning Calorimetry (DSC), etc.

The Cs-Mo-O system is of fundamental importance because Cs2MoO4 is expected to be the main component of the JOG. A CALPHAD assessment of the Cs-Mo-O system has been performed in the frame of the TAF-ID project (Thermodynamic of Advanced Fuels International Database [3]), based on the limited experimental data available in the literature. Because this system is very complex, many fundamental thermodynamic properties are still missing, and discrepancies have been noticed. The Cs-U-O system is another key system for modelling the JOG, as Cs2UO4 is the main phase on the pellet-side of the JOG layer. A Cs-U-O CALPHAD model has been developed in the TAF-ID on the basis of the review of Cordfunke and Konings [4], but discrepancies in the literature exist for this system and thermodynamic data are missing for some of the key phases, in particular CsUO3.5. Finally, the data available on Cs-Te-O are rather scarce, and no thermodynamic model has been reported to this date. A particularly interesting study is the investigation of the solubility of Te in Cs2MoO4, which is reported herein.

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Poster flash talks / **25**

Thermodynamic modelling of the U-Pu-Am-O system

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The thermodynamic modelling of the U-Pu-Am-O system is proposed by using the CALPHAD method. The aim is to provide basic thermodynamic data (melting temperature, heat capacity ⋯) on the (U,Pu,Am)O2 mixed oxide fuel to be used as input data in Fuel Performance Codes. In 2011, a CALPHAD model was developed in the TAF-ID database. An update of some of the binary and ternary sub-systems is proposed on the basis of a review of available recent experimental and/or theoretical thermodynamic and phase diagram data. The calculated results with the updated model will be compared to the experimental data.

Poster flash talks / **55**

Advances in phase-field modelling incorporating bulk thermodynamics and interfacial excess quantities

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This work discusses advances in phase-field modelling of multiphase nuclear materials with a focus on incorporating bulk equilibrium thermodynamics and interfacial phenomena. Tools have been developed for the automated construction of explicit multiphase, temperature dependent composite potentials from those of the pure phases obtained from CALPHAD-type databases. The interfacial energy is explicitly controlled and permits consideration of interfacial excess quantities permitting structurally-semicoherent interfaces. This work extends the applicability of bulk thermodynamics to systems dominated by interfacial effects such as nanoscale systems, and kinetically limited, non-equilibrium scenarios. Applications for precipitation of zirconium hydride in fuel cladding, and the evolution of fuel porosity are discussed.

Poster flash talks / **46**

Adaptive Kinetic Monte Carlo (AKMC) modelling of radiation defects in mixed oxide (MOX) fuel

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Atomistic modelling of materials is typically achieved by using Molecular Dynamics (MD). However, due to the fact that MD needs to resolve atomic vibrations, a very large number of small time steps are needed and the total simulation time is therefore often limited to less than one microsecond. The timescale limitation can be overcome by using Adaptive Kinetic Monte Carlo (AKMC) methods. Kinetic Monte Carlo methods exploit the fact that over longer time periods the dynamics of atomic systems typically consist of diffusive jumps from state to state.

We have used the Daresbury laboratory AKMC code (DL-AKMC) to explore the possible atomic transitions (and associated energies) of a 30% Pu MOX structure with five different types of cation Frenkel Pair defects at 1020K, 1600K and 2170K. The Potashnikov interatomic potential was used throughout this work. The software package Ovito has also been used to visualise and map atom movement. We present a statistical analysis of the atomic transitions and discuss how these can be used as a starting point for understanding the evolution of radiation damage in MOX fuel.

Poster flash talks / **36**

A new laser heating setup for the measurement of noble gases diffusion in nuclear materials

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The noble gases helium, krypton and xenon are generated or implanted in many materials employed in or developed for fission or fusion nuclear reactors (e.g. UO2, neutron absorbers, high-level waste matrices, etc.). Taking the example of the usual fission nuclear fuel UO2, the in-pile generation of noble gases is greatly responsible for the unfavorable microstructure and thermal properties evolutions of the fuel. However the underlying mechanisms governing the behavior of these gaseous elements in UO2 are so far not entirely understood and are almost unknown for the GenIV fuel candidates. Consequently, the diffusion mechanisms and kinetics of noble gases in nuclear materials are paramount to determine for a comprehensive range of experimental parameters. These are however often quite complex to access experimentally, especially when looking to low concentrations to avoid the formation of gas bubbles or defect aggregates.
At our laboratory the quantification of noble gases diffusing out of materials is made possible down to as low as few 107 atoms thanks to advanced gas purification and mass spectrometry techniques. However our investigations were up until recently limited by the actual conventional vacuum furnace used for samples heating (maximum temperature of 1400℃, imprecise control of temperature, impossibility to control and impose oxygen partial pressure (pO2), etc.).
To overcome these limitations, a new heating line has recently been implemented. The latter is based on the use of a high-power laser beam able to quasi-instantaneously and homogeneously heat the samples to controlled temperatures in the range of 600 to 2200℃, with a limited heating of the sample holding components. Furthermore we are currently trying to implement a pO2 control system to be able to vary this crucial parameter.
The proposed poster aims to present the features of this new experimental line and the unique new possibilities of investigation brought by this new setup. A recent example study will also be presented: helium diffusion mechanisms and kinetics in B4C.

Poster flash talks / **39**

Sintering behaviours and microstructure analysis of UN-UO2 composite fuels prepared by spark plasma sintering

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Uranium mononitride (UN) has been considered a potential accident tolerant fuel (ATF) mainly because its high uranium density, high melting point, and high thermal conductivity. Composite fuels like UN-UO2 have been proposed so as to combine the good properties of both fuels. This study is focused on analysing the first results regarding the sintering behaviours and the microstructures of an innovative UN-UO2 composite fuel concept, prepared by mixing UN microspheres with UO2 powder followed by spark plasma sintering (SPS).
Pure UO2 powder, 30 wt.% of UN microspheres in UO2, and pure UN microspheres were sintered using SPS at 1100ºC and 1500ºC. The UO2 powder used in this study was provided by Westinghouse Electric Sweden AB. The UN microspheres were fabricated at Chalmers University of Technology by internal sol-gel method, with a chemical composition of U(N0.98C0.02) (a = 4.8904 Å, TD = 14.31 g/cm3) and density of about 52 %TD.
The sintering behaviours of UO2(1100ºC) and UO2(1500ºC) were similar. The shrinkage started and finished at 450ºC and 900ºC, respectively, with a characteristic "S shape"sintering curve. Conversely, the sample UN(1500ºC) started to sinter at approximately 1100ºC and was still densifying at 1500ºC. Regarding the composites, the initial behaviours were similar to pure UO2 until about 600ºC. Afterwards, there were a sintering blockage in both samples up to ˜900ºC, where the shrinkage rates started increasing again.
The sintered densities were measured using a modified Archimedean method with chloroform as the medium. For UO2(1100ºC), UO2(1500ºC), UN-UO2(1100ºC), UN-UO2(1500ºC), and UN(1500ºC) densities above and around 90 %TD were achieved. Additionally, the microstructure analysis are presented and discussed in this study.
This work shows that it was possible to fabricate an innovative UN-UO2 composite fuel concept by SPS. The preliminary results of the sintering behaviours show that the UN microspheres supressed the UO2 matrix densification in both UN-UO2(1100ºC) and UN-UO2(1500ºC) samples. This fact might be related to the UO2-UO2 particle separation by the addition of 30 wt.% of UN, impairing the stage where neighbouring necks grow and interact to give a network of tubular pores. Moreover, the UN microspheres alone also sintered when the temperature is higher than 1100ºC. Additional studies are under development in order to better understand the UN/UO2 interaction during sintering.

Poster flash talks / **10**

Microstructural investigation of (U,Pu)O2-x fuel by Raman spectroscopy

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For the future Sodium-cooled Fast Reactors, uranium-plutonium mixed dioxide (U,Pu)O2-x, with the plutonium content ranging between 19 to 40 mol.%, is foreseen as potential fuel. The pellets have to match various physico-chemical specifications: physical integrity, chemical homogeneity, to be

oxygen hypostoichiometric (Oxygen/Metal ratio included in 1.94 and 1.99 range). However, for a Pu content higher than 20 mol.%, and an O/M ratio lower than 1.98, at room temperature, the phase diagram of U-Pu-O system exhibits a miscibility gap domain [1]. The sample is then composed of two phases of same structure but different O/M ratios. The detailed consequences of this demixtion phenomenon, such as formation of cracks and its kinetics has to be fully investigated.
Recently, Talip et al [2] and Elorrieta et al [3] have evidenced that Raman spectroscopy is a promising tool for characterizing (U,Pu)O2 materials. This technic is based on the interaction of a monochromatic light, usually a laser, with the matter. Coupled with a microscope, this technique can be used to determine several physico-chemical properties at the grain scale (˜5 µm). For instance, information on crystallographic phases, chemical homogeneity, grain size, and crystal defects can be directly obtained.
UO2, PuO2 and (U,Pu)O2 share the same Fm-3m structure and consequently their Raman active modes are identical, but appear at different wavenumbers in their respective spectra. The main Raman band is the T2g which corresponds to the asymmetrical stretching of the O-O bonds. Its position gives information on the O/M ratio and on the Pu content in (U,Pu)O2±x mixed oxides. Moreover, as showed by Maslova et al [4] using UO2 disc samples, the T2g intensity is directly related to the grain orientation. As the size of the laser beam used is micronic, the observation of porosities and grains is then possible when mapping the surface of the sample, thus revealing its microstructural features.

In the present work, this technique has been extended to (U,Pu)O2.00 fuels. Using a similar approach existing in the literature [4], the (U,Pu)O2 sample microstructure has been studied using µ-Raman imaging technics.
Furthermore, the T2g Raman band mapping on large area of our samples allows us observing µm2 scale heterogeneities in the Pu content.
As this characterization tool was first used on samples with an O/M ratio equal to 2.00, we have extended the method to oxygen hypostoichiometric materials. By using both in-situ and ex-situ thermal treatments with a dedicated device [5] allowing a precise oxygen partial pressure control, various O/M ratios could be achieved. The study of the variations in the (U,Pu)O2 fuel microstructure according to both the Pu content and the O/M ratio is now possible and our first results will be presented.

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Poster flash talks / 106

Simulation of pure and Cr-doped UO_2 using molecular dynamics and density functional theory

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Uranium dioxide (UO_2) is an important industrial material which is employed as a fuel in most nuclear reactors world-wide. The doping of UO_2 with small amounts of chromium oxide Cr_2O_3 is technically applied to obtain a larger average grain size after the fuel sintering process. In this study the local environment of chromium in UO_2 was investigated using X-ray absorption spectroscopy. An interpretation of the X-ray absorption spectra is a non-trivial task, especially for so complicated systems like doped fuel. Here we will address this challenging problem using two approaches, in which the ab initio EXAFS theory is combined with classical molecular dynamics (MD) or ab initio

molecular dynamics (AIMD) as well as electronic structure simulations based on density functional theory (DFT). The atomic scale MD and DFT simulations were carried out using the CP2K code. Alternatively, DFT simulations were performed to determine the influence of the chromium doping on the fuel matrix. The atomic structure around the chromium impurity was relaxed, and the resulting structures were used to calculate the Cr K-edge EXAFS spectra. The comparison of the simulated EXAFS spectra derived from DFT results with the experimental one allows the identification of valid atomic configurations. The limitations of this approach are discussed.

Session 5 / **4**

Postirradiation Examination on Innovative Advance Reactor Metallic Fuel Concepts

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In sodium fast neutron spectrum nuclear reactors, metallic uranium-based alloys have often been chosen because of their high fissile density, high thermal conductivity, and several reactor kinetic safety benefits. In order to address increasingly high burnup / high performance demands, a number of innovative design are under investigation within the Department of Energy's Advanced Fuels Campaign (AFC). As part of this development, candidate fuel compositions and forms are irradiated in a cadmium-shrouded positions at the INL's Advanced Test Reactor (ATR), and they are subsequently examined at the Hot Fuel Examination Facility (HFEF).
Historically there were two primary factors that limited the life and maximum temperature of metallic fuel. At burnup greater than 20 atomic percent, solid fission products began to fill the porosity in the fuel resulting in fuel pin swelling. At high burnup and high operating temperatures, fuel cladding chemical interaction (FCCI) occurs where lanthanide fission products attack the cladding reducing the effective cladding thickness. To mitigate these performance factors, the evaluated innovative fuels design fall into four categories alternative alloying metals, additives, sodium bond removal, and alternative smear densities. For alternative alloys, Zr has been substituted for 10% Mo or 5% Mo, 4.3%Ti, 0.7%Zr to stabilize the cubic phase of U and prevent constituent redistribution seen in U-Zr alloys. Additives, such as Pd, have been suggested to bind lanthanide fission products, effectively reducing FCCI. Sodium bonding is considered undesirable at the back end of the fuel cycle where sodium bonded fuel must be treated to remove sodium prior to geological disposition. Helium bonded metallic fuel of several alloys has been irradiated to better understand the implications of removing sodium bonding. Low smear density fuel is necessary to enable high (30 at.%) burnup. Both solid and annular low smear density fuels have also been examined.
Engineering scale postirradiation examination (PIE) and microstructure scale PIE results will be presented and discussed for the different categories of innovative fuel designs.

Session 5 / **19**

Study of alpha self-irradiation on americium-doped uranium oxide

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The transmutation of minor actinides in the future generation of fast-neutron nuclear reactors is an option to decrease the volume and the overall radiotoxicity of the nuclear fuel inventory. Within minor actinides, americium is the one having the highest radiotoxicity. Several scenarios are considered for introducing it back into the core of nuclear reactors, either homogenously distributed in the nuclear fuel, or heterogeneously loaded in minor-actinide bearing radial blankets.

Due to its high alpha activity, americium strongly increases the alpha dose received by the fuel over time. For this reason, many studies focused on the effect of alpha self-irradiation in americium bearing materials. Here, we present results obtained on UO2 samples doped with 241Am at 5 at.% level. The samples were prepared by a sol-gel co-precipitation method ensuring a homogeneous starting material. The work mainly focuses on the effect of alpha self-irradiation on the low-temperature specific heat, which in pure UO2 is characterised by a large anomaly at 30.8 K signalling a first-order magnetic transition. While self-irradiation damage accumulates with time, the anomaly shifts to lower temperature and broadens as the phase transition becomes discontinuous. The study is complemented by a characterization of the time evolution of the material microstructure through powder X-ray diffraction, transmission electron microscopy, and Raman spectroscopy.

Session 5 / **23**

Accelerated Testing of Fast Reactor Fuel in the Advanced Test Reactor

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Idaho National Laboratory has a long and internationally recognized history of performing irradiation testing of advanced fast reactor fuels in the Experimental Breeder Reactor II (EBR-II) and the Advanced Test Reactor (ATR). Since EBR-II's decommissioning in the early 1990's, irradiation testing has been exclusively performed in ATR. The testing of fast reactor fuels in ATR is challenging given its thermal neutron spectrum and coolant temperatures far below those prototypic of fast reactors. Researchers have overcome these obstacles through the use of Cadmium shrouds which attenuate all thermalized neutrons and an experiment design that fosters fuel and cladding temperatures prototypic of fast neutron reactors. Although this design has successfully demonstrated temperatures and temperature gradients that closely mimic those seen in fast reactors, irradiation performance is highly sensitive to fabrication tolerances and the time requirements necessary for high fuel burnup, where irradiation performance data of fast fuel is lacking, are significant. This work summarizes two novel experiment designs and their associated physics analyses for testing fast reactor fuels in ATR; an accelerated irradiation experiment and a fast spectrum experiment. The accelerated irradiation experiment does not utilize a Cadmium shroud and has been shown to triple the burnup rate, yet still yields temperatures and radial power profiles prototypic of fast reactor fuels. The fast spectrum experiment utilizes a booster fuel element that that hardens the incident neutron spectrum and also yields temperatures and radial power profiles prototypic of fast reactor fuels. These experiment designs efficiently reduce irradiation time requirements, are more economical, and significantly increase ATR throughput. Fast reactor experiments that capitalize on these designs expedite irradiation performance data for fast reactor fuels and provide information invaluable to fuel performance modeling and simulation validation over a wide range of parameters.

Session 5 / **48**

In-Pile Experiment Development to Investigate Transient Irradiation Performance of Fast Reactor Fuels at TREAT

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Transient irradiation testing of fast reactor fuels has been a major emphasis of several historical programs supporting both oxide and metal fuels for sodium-cooled fast reactors. These programs have been executed at several test facilities around the world, though today, very few remaining facilities exist capable to perform such studies. The purpose of these programs is to understand and establish fuel performance limits under anticipated off-normal, design basis, and beyond design basis accident conditions. The recent restart of the Transient Reactor Test (TREAT) Facility in the U.S. has provided unique capability and established renewed efforts to study advanced fuels under transient conditions. While water testing is already underway, test designs are rapidly maturing to support testing of advanced liquid metal cooled fast reactor fuels. These test designs include a liquid sodium capsule and a flowing liquid sodium loop. Detailed design efforts are underway to provide flexible testing environments that include advanced instrumentation to quantify fuel performance in a manner never previously performed. Nominally the experimental devices will support metal and oxide fuels for sodium-cooled faster reactors with logical extension to other fuel designs as needed. In the U.S., test plans for metal fuels are maturing to extend the existing fuel performance database and provide opportunity to evaluate novel fuel designs. These tests are also designed to leverage a large inventory of irradiated fuel pins from the Experimental Breeder Reactor (EBR)-II and Fast Flux Test Facility (FFTF) s that remain in storage on the INL site (both metal and oxide forms). This presentation will provide a detailed overview of the planned program and current status of test design and predictions for fuel performance.

Session 6 / **54**

Mesoscale fission gas percolation simulations of heterogeneous and irregular grain networks

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The two-species Included Phase Model (IPM) has been utilized to simulate percolation of grain boundary fission gas bubbles on two-dimensional hexagonal grids representing (U,Pu)O2 fuel. Simulations were performed in which transport of vacancies and fission gas were coupled with minimization of internal, elastic and interfacial energies on networks of 15-300 grains with a computationally efficient mesoscale technique. An open surface at a boundary allows gas venting and subsequent tunnel collapse. The impact of the stochastic nature of compositional heterogeneity and irregular grain size on macroscopic fuel performance behaviour was explored statistically by analyzing the results of a series of randomly generated cases. The macroscopic fuel performance properties: grain boundary concentration, fission gas release fraction, vacancy fraction, and fractional coverage were analyzed for each case.
Compositional heterogeneity in Mixed Oxide fuel was simulated by randomly distributing plutonium-rich, high fission density grains on a regular hexagonal grid, the proximity of which to the free surface was found to dominate the percolation behavior. Irregular grain size was simulated on equiangular hexagonal grains with irregular edge length and grain area. An analysis of individual edges showed discrete growth modes corresponding to the number of fission gas bubbles which nucleate on each edge. For edges in the bulk, percolation time is most strongly correlated to the edge length, then to a lesser degree grain area and proximity to the open surface.

Session 6 / **44**

3D-reconstruction via genetic algorithms: Application to metallic fuel

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Inferring 3D features of heterogeneous materials (e.g., solid materials with gaseous porosity) from 2D sections is the subject of stereology. This inference process is critical for the determination of various and fundamental properties of the 3D medium, such as the pore size distribution and the percolation thresholds. Stereological approaches have been tailored to different materials/properties, but lack of generality and depend on very strong hypotheses. In the attempt to overcome these limitations and allowing to approach a broader range of material/properties, in this work we present a 3D reconstruction technique leveraging a genetic algorithm. The 3D-reconstruction problem is treated as an optimization problem: a population of virtual 3D cubes –embodying a certain void fraction –is randomly generated and selected by comparing cubes sections with a reference 2D image in terms of specific optimization metrics (e.g., the number of pores and the pore average radius). Once the population of 3D cubes is optimized by the genetic algorithm (i.e., it is possible to extract from it a population of 2D sections comparable with the reference image), it can be used to determine correlations between 2D (measurable) quantities and 3D (to be inferred) quantities. Moreover, since the outcome of the genetic algorithm is not a single optimal 3D cube, but a whole population of cubes, confidence intervals can be derived for these correlations. The proposed approach is very broad and general, applicable in many specific topics related to nuclear fuel (e.g., high burnup structure, grain growth, porosity development, and so on). In this work, we showcase the application of the proposed 3D-reconstruction algorithm to a subset of fuel sections of metallic fuel obtained as part of the post irradiation examination of the FUTURIX campaign, with focus on the development of porosity. The goal is to demonstrate the applicability of the proposed algorithm to the 3D-reconstruction of metallic fuel, in terms of total porosity, porosity-2 and pore-size distribution.

Session 6 / **24**

A DEM/FFT approach to compute the effective thermal conductivity of fragmented fuels under accident conditions

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Simulation of the effective properties of granular media such as thermal conductivity is of a great interest for many applications. Under accident conditions the nuclear fuel may crack and relocate inside its cladding. In this case, the relocation leads to a degraded conductivity of the fuel. Thermal conductivity evaluation is interesting to evaluate the temperature in the fuel rod.
We developped a chained method involving Discrete Element Method (DEM)[1] and Fast Fourier Transform (FFT)[2] : We first compute the packing microstructure,
according to the grains kinetic, with DEM. The microstructure is voxelised and finally the FFT method is employed to compute the effective thermal conductivity of the granular media. This method allows us to compute accurately the effective thermal conductivity of a granular media taking its real microstructure into account.
We also performed a sensitivity analysis over the discretisation parameters, the size of the seed as well as the definition of interfacial voxels having both solid and gas phases (called fuzzy voxels). Thus we propose to define several bounds and estimates of the effective thermal conductivity depending on the definition of the fuzzy voxels. Finally, we compare the results of the DEM/FFT method to experimental measurements available in the litterature[3, 4] and show a good agreement between our simulations and the measurements.

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Session 6 / **28**

Development and assessment of a mechanistic model describing high burnup structure behavior in oxide nuclear fuel

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The combination of high burnups and low temperatures occurring in the rim of oxide fuels, or in plutonium-rich islands of heterogenous mixed-oxide fuels, leads to a re-crystallization of the as-fabricated microstructure. The resulting structure, known as high burnup structure (HBS), is featured by nanometric-size grains and may develop substantial porosity as burnup proceeds. These aspects strongly affect the performance of oxide fuels in normal operating conditions and may jeopardize the integrity of the fuel rods during accidental transients (e.g., LOCA) at high burnups. Thus, developing models to be included in fuel performance codes is of the utter importance for a more reliable simulation of fuel rod behavior at high burnups. In this work, we present a mechanistic model describing the formation and evolution of the HBS in oxide fuels, featured by a level of complexity suitable for application in fuel performance codes. The model includes a semi-empirical modelling approach to HBS formation, expressing the volumetric portion of restructured fuel as a function of local effective burnup (i.e., the burnup accumulated below 1000℃) by the Kolmogorov-Johnson-Mel-Avrami (KJMA) relationship for phase transitions. The KJMA parameters were fitted combining experimental data on restructured volumes extracted from [1, 2] with TRANSURANUS simulations for the estimation of local effective burnup. We used the ImageJ image analysis software to derive novel data from [2]. The evolution of the HBS intergranular porosity is accounted for in a mechanistic fashion. Starting from the cluster-dynamics master equations governing the problem, we apply a Fokker-Planck expansion of the master equations in the cluster size space. In doing so, we derive a single-size model that describes not only the time-evolution of HBS pores number density, but also the first (mean size) and second (variance) moments of the pore size distribution. The model accounts for HBS pore growth due to the capture of fission gas atoms diffusing from the restructured HBS grains, and for pore-size-dependent irradiation re-solution. Moreover, pores are assumed not to be in mechanical equilibrium and can thus relax overpressure by absorbing vacancies. Pores interconnection by impingement during growth is accounted for, assuming pair interactions of HBS pores treated as monodispersed hard spheres [3]. We implemented the model in the SCIANTIX gas behavior code [4] and compared the calculation results to available experimental data in terms of xenon depletion in the fuel matrix [5], to models available in the open literature, and to data on HBS pore number density, average radius, and resulting fuel swelling [6]. Model results demonstrate a good agreement of model predictions with the experimental data and considered models from the open literature, on both xenon depletion and porosity evolution, together with computational burdens in-line with fuel performance codes requirements.
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Session 7 / **41**

New insight into the thermodynamic and atom transport properties of (U,Pu)O_2 nuclear fuel from atomic scale calculations

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The uranium-plutonium mixed oxide (U,Pu)O_2 is currently used as nuclear fuel in pressurized water reactors with a Pu content around 10 wt.%, and is the reference fuel for several Generation IV reactors with a Pu content between 25 and 40 wt.%. A more precise knowledge of the properties of (U,Pu)O_2 and its behaviour under irradiation is needed to refine the models used in the fuel performance codes simulating the behaviour of fuels at the macroscopic scale. A basic research approach coupling detailed characterizations and multiscale modelling starting at the atomic scale can bring significant insight into key phenomena involved in the evolution of nuclear fuels during their reactor life.
We will show the results obtained using state-of-the art electronic structure calculations, including ab initio molecular dynamics simulation, and empirical potential methods on thermodynamic and atomic transport properties of (U,Pu)O_2. In particular, the thermal expansion, mixing enthalpy and specific heat of (U,Pu)O_2 as a function of Pu content will be discussed in view of the available experimental data. The defect properties of (U,Pu)O_2 with 25% Pu as a function of the oxygen-potential will also be presented.

Session 7 / **14**

Development of a thermo-kinetic model of cations in the mixed oxide of Uranium & Plutonium

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The large radial thermal gradient in Sodium-cooled Fast reactors (SFR) leads to mass transport of uranium and plutonium in the fuel pellet. Knowledge of self-diffusion of all these elements in (U,Pu)O2 fuel is therefore of utmost importance for the prediction of its in-pile behaviour. Very few experimental data, however, are available on self-diffusion in this material.

In the inception of the study, the lack of experimental measurements is circumvented by the so-called 'cBΩ'model. The cBΩ model has been utilized to describe the plutonium self-diffusion in MOx using the bulk properties of the fuel and a single fitting-parameter.

Using these results of cBΩ and the experimental data together, a plutonium mobility database has been composed for the MOx fuel. Hence, by implementing this database, a detailed model has been developed to describe the plutonium self-diffusion in MOx using the state-of-art DICTRA code.

The self-diffusion of Uranium in MOx has not been experimentally measured yet. However, by implementing the thermodynamic definition of MOx and the plutonium self-diffusion model, developed under this work, the self-diffusion of Uranium has been estimated from the experimentally measured cation inter-diffusion coefficient data. Hence, a similar Uranium mobility database for

MOx has been also composed. Further, using this database, a model for the uranium diffusion in MOx has been developed.

Both the models for self-diffusion of Uranium and Plutonium has been validated against the experimental results. In combination of these two models of cation self-diffusion in MOx, the inter-diffusion profile of cations has been simulated.

Session 7 / 35

Assessment of the current European Fuel Performance Codes against the Fast Reactor irradiation experiment SUPERFACT

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This work is devoted to the first assessment of the state-of-the-art European fuel performance codes GERMINAL, MACROS and TRANSURANUS against integral and microscopic data from post-irradiation examinations in the fast reactor irradiation experiment SUPERFACT. This activity is performed by a Task Force, including CEA, JRC, ENEA, SCK.CEN and POLIMI, in the framework of the H2020 European Project INSPYRE. The goal of the experiment was to study how mixed oxide fuel (MOX) containing the minor actinides neptunium and americium behaves under irradiation in a fast reactor, and to demonstrate the feasibility of transmutation of minor actinides through homogenous (i.e., low minor actinide content) and heterogeneous (i.e., high minor actinide content) fuel concepts.

Two types of homogenous-concept fuel pins from the SUPERFACT-1 experiment were selected for this work, more precisely the pins SF7, SF13 bearing 2 wt.% of 237Np, and SF4, SF16 bearing 1.8 wt.% of 241Am. Their plutonium content (around 25 wt.%) and cladding material (15-15, titanium stabilized, cold worked stainless steel) are in line with the characteristics envisaged for Generation-IV reactor fuels. The current predictions of the codes are compared to experimental data from non-destructive and destructive post-irradiation examinations. The integral data considered for validation are: final burn-up at peak power node, fission gas (xenon and krypton) production and release, helium release, central hole axial extension, and fuel and cladding elongations. Further local measurements were made by cladding profilometry, as well as for the fuel central void radius and for the extension of the columnar grain region. Finally, microscopic data are available for the radial distributions of the minor actinides 237Np and 241Am, as well as of plutonium, xenon and caesium.

The overall agreement with experimental data is acceptable but reveals room for improvement and highlights discrepancies between code results. The analysis is complemented by a code-to-code benchmark, focusing on the evolution of relevant output quantities over time (e.g., fuel central temperature, fuel-cladding gap width, cladding outer radius, rod internal pressure, and fission gas release).

The goals of this analysis are to assess the current capabilities of fuel performance codes and to underline modelling gaps through the differences among computations and experiment, benchmarked with different codes. This is fundamental for identifying possible common development areas and for improving the prediction of MOX fuel behaviour in fast reactor conditions. Indeed, improved fuel performance codes will allow for a better performance and safety analysis of next Generation-IV fast reactors (e.g., MYRRHA, ASTRID, ALFRED), and will play a key role for the definition of their final design and future development.

Session 7 / **53**

Modelling of the H2020 INSPYRE fuel creep experiment in HFR with TRANSURANUS

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The fuel creep experiment is currently being prepared within the H2020 INSPYRE project for irradiation in High Flux Reactor in Petten. The goal of this experiment is to produce in-core online measurements of dimensional changes of UO2 and MOX fuel samples under applied axial load.
In this work TRANSURANUS (TU) Fuel Performance Code in combination with Finite Element Analysis (FEA) is used to model the fuel creep irradiation experiment in great detail. The thermal analysis of the experiment is carried out using the FEA. Such approach enables to model a rather complex geometry of the experiment, and to include axial heat transport (not implemented in TU).
The TU is modified in order to use the externally calculated with the FEA temperatures, and to include the axial load present in the experiment. The TU provides the FEA with fuel pellet dimensions and temperature and burnup dependent fuel properties.
The developed model is used to predict the fuel behavior using a selection of foreseen irradiation scenario's. The results will be used for optimization of the irradiation parameters and for data analysis.

Session 8 / **38**

Thermodynamic properties of Fe-Zr-O system at high temperatures

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The Fe-Zr-O ternary system is essential in order to estimate the possible material interactions during a severe accident of nuclear power plant. In the reactor vessel, the core losing its cooling ability drives temperature escalation due to decay heat, leading to the onset of U-Zr-O melt formation about at 2173 K which is 1000 K lower than the melting point of UO2. The melt can go through the steel structures into the lower plenum involving the interaction between Fe and U-Zr-O. Quenched melt in the lower plenum will be heated up again by its decay heat accompanied with further interaction with peripheral steel structures. In order to see the effect of these chemical interactions between Fe and U-Zr-O alloy, we performed the preliminary calculation of heat generation from the reactions using TAF-ID database. Consequently, it was found that the interaction of Fe with Zr-O rich alloy could produce several times of latent heat for Fe even if several percent of Fe is added in the system. The heat source of reaction comes from the Zr-rich oxide precipitation driven by Fe addition and this indicates that assessment of Fe-Zr-O system is critically important to improve accuracy of prediction. However, the current database has been optimized using the interaction parameter only for Fe-rich Fe-Zr-O mixture. Experimental evaluation of thermodynamic properties for Zr-rich mixture is necessary for the severe accident analysis. We propose a measurement of thermodynamic properties by a chemical equilibrium technique. Principle of "identical chemical potential in equilibrium state"enables us to determine Gibbs free energy of formation of compounds, the activity of components, elemental absorption ability of the system, Gibbs free energy of dissolution of oxygen into the system and mixing enthalpy through activity coefficient determination. The experimental apparatus consists of an electric resistance furnace connected to the gas control lines. The Fe-Zr mixture is put inside the ZrO2 crucible and temperature is kept until the material reaches the equilibrium

state. The cooled material at the end of test will be chemically analyzed to obtain a concentration of component, which is the basic data for calculating thermodynamic properties. The experiment is planned for temperature above 1800 K and a wide variety of composition from 1wt% ˜ 90 wt% of Zr.

Session 8 / **32**

Experimental investigation of the U-Zr-Fe-O liquid miscibility gap

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The U-Zr-Fe-O system is of paramount importance for severe accident studies on light water reactors. This chemical system is characterized by a miscibility gap in the liquid phase. This means that two liquids, one metallic and one oxide, can coexist in a wide range of temperature and composition. Experimental data on this miscibility gap are rare: experimental difficulties related to the complex behavior of this system at high temperature (reactivity with crucibles, control of the oxygen potential, vaporization) have limited the amount of data available in literature. In the frame of the INSPYRE project, CEA started an experimental campaign using the ATTILHA setup. This setup is based on a laser heating technique that can be coupled with an aerodynamic levitation system. Pyrometers and an infrared camera are used to monitor the temperature and the thermal behavior of the samples. This configuration allows to limit the interaction between the sample and the surrounding materials, e.g., with the crucible. Furthermore, it allows to reach extreme temperature conditions (T>2500 ℃) in a controlled atmosphere.
Starting from metallic alloys, the setup allowed to progressively oxidize the samples while heated and therefore enter into the metallic-oxide liquid miscibility gap. After the target temperature and composition were reached, the sample was quenched to room temperature. SEM-EDS and EPMA analyses were then performed to obtain the composition of the solidified liquids in equilibrium.
The current work focused on the liquid miscibility gaps of three subsystems: Fe-O, Fe-Zr-O and Fe-U-O. Tie-lines have been obtained for these systems for different temperatures. Also, thermodynamic calculations using the TAF-ID database were performed to help the interpretation of the experimental results. Finally, these novel experimental results will be used to feed the TAF-ID thermodynamic database.

Session 8 / **42**

Physico-chemical properties of molten salt fuel: development of innovative techniques

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In order to support the constant improvement of nuclear technology, the Molten Salt Fast Reactors (MSFR) were proposed satisfying the main goals of the Generation IV Nuclear Reactors as sustainability, safety and reliability, economic competitiveness and proliferation resistance. The peculiarity and innovation of the MSFR technology is the use of liquid fuel, a molten salt mixture in which fissile and fertile isotopes are dissolved. The knowledge of physical properties as density and viscosity of the molten salts is required to predict the flow and turbulent heat transfer of the fuel through the reactor circuit since it serves the dual function of nuclear fuel and heat transfer medium. Due to the small amount of salt usable, the radioactivity of the samples, their corrosiveness, and high temperature current techniques for determining these properties cannot be used with molten salts. An innovative method based on ultrasonic wave propagation has been developed for the determination of the viscosity of fluids at high temperature. A waveguide is used to remotely transmit the ultrasonic waves from a shear piezoelectric transducer into the molten salt. At the solid–fluid interface, a guided wave mode, the shear mode, is used to extract the fluid properties. The ultrasonic wave energy reflected back depends upon the operating frequency, the physical properties of the fluid (viscosity and density), and the waveguide (density and shear modulus). The results show that the attenuation of the waves can be retrieved using this method. Measurements on water, ethanol, oil and glycerine-water mixtures illustrate that the method can successfully monitor changes in attenuation due to the viscosity of the fluid. The range of viscosity measured was between 1 and 40 mPa s, since this is the same predicted range of viscosity of molten fluoride salts at various temperatures. The fluids are measured at a variable temperature between 20 and 30°C showing a decrease in the viscosity with temperature as expected. The relative error for these measurements was always lower than 5% and it is believed to be mainly due to geometrical features of the current experimental setup. An ionic salt with very similar properties to the molten salt was measured. The error was in this case 20 % and it is believed to be due to particular properties of ionic salts to be investigated. A set up for measuring fluids up to 100°C is under development and it will be followed by the construction of a furnace for molten salts.
This method offers advantages in measuring viscosity reducing experimental time and using a small amount of sample without any mechanical equipment.

Session 8 / **31**

High temperature interaction between UO2, steel and B4C in the frame of sodium fast reactor severe accident studies

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The Sodium Fast Reactor (SFR) is one of the reference reactor among generation IV nuclear systems. The investigation of severe accidents is essential for the design of SFR reactors. In fact, during a severe accident, the MOX fuel, steel cladding and B4C neutronic absorbers can interact forming a complex mixture of gas, liquid and solid phases. In order to predict the phase equilibria at high temperature, the development of a thermodynamic database on the (U-Pu-O)-(Fe-Cr-Ni)-(B-C) system is required to perform thermodynamic calculations. To provide input data for the modelling, an experimental thermodynamic study is carried out.

In a first test, where mixed powders of UO2, B4C and small pieces of Fe have been mixed and heated at 1900℃ for one hour, we have shown that UO2 has been reduced by B4C to form U-Fe-B and U-Fe-C ternary compounds. These compounds will have to be introduced in the CALPHAD model. To study the effect of the steel alloying elements (Ni and Cr), a heat treatment has been performed in the same conditions (1900℃ for one hour) on a sample made by arc melting from B4C, steel and UO2. The chemical composition of the phases have been measured by EDS and EPMA.

In addition, in order to be closer to the real fuel materials geometry and to study the kinetics of the reactions at the materials interfaces, diffusion couple tests on UO2 pellet / steel cladding / B4C pellet samples have been performed at temperatures below 2000℃ and for several durations (maximum 7 hours). In these experiments, Knudsen Cell Mass Spectrometry has been used to follow the gaseous species release during the reactions. All these results will allow to conclude on the deviation from thermodynamic equilibrium conditions and to assess the reaction kinetics.

Session 9 / **9**

Manufacture and modelling of advanced UB2 fuel

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The manufacture and modelling of UB_2 has been carried out to understand its suitability for use as a fuel within light water reactors. Density functional theory methods have been used to understand the materials thermal properties and response to radiation, fission product accommodation and impurities. This theoretical work has been combined and elevated with a targeted experimental programme highlighting synthesis routes for UB_2 and the related ZrB_2 compounds and providing experimental data to validate and verify the theoretical predictions.

Session 9 / **26**

Interaction between sodium and nanosized mixed oxide fuel (U1-xPux)O2: focus on the structural characterization of Na4(U1-xPux)O5.

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The mixed oxide (U1-xPux)O2 is currently the reference fuel for the Sodium-cooled Fast Reactors. In case of severe accident, the irradiated fuel would interact with the sodium in a large temperature

range. In order to assess the safety of the Sodium-cooled Fast Reactor, the study of the Na-U-Pu-O system is mandatory. In previous studies [1] [2] [3], some compounds have been reported but no thermodynamic data exist on the quaternary phases and the synthesis of pure phases was challenging.
In this work, we used the oxalate decomposition under hot compressed water at low temperature [4] to get the starting materials (U1-xPux)O2 (x= 0.06, 0.13, 0.29, 0.46). Thanks to this new way of synthesis, the mixed oxide fuels produced are nano-sized and have a spherical shape instead of plate-like agglomerates [5] [6]. Moreover, they are more reactive than the previous compounds, facilitating the synthesis of pure phases.
These nanocrystals were mixed with different amounts of Na2CO3 or NaOH to explore which compounds will be formed. Along this talk, the first results on the interaction between nano-sized mixed oxide fuels and sodium will be presented. Especially, we have obtained pure Na4(U1-xPux)O5 which has been analysed by X-ray powder diffraction (XRD) and U M4/Pu M5 high-energy resolution X-ray absorption near-edge structure (HR-XANES) spectroscopy. Analysis of the XRD patterns demonstrate that the lattice parameters are not following the Vegard's law between Na4UO5 and Na4PuO5. As expected from the structure of the ternary compounds, the HR-XANES spectra show that uranium is in a +VI oxidation state whereas the plutonium has a lower oxidation state. This would explain the deviation from Vegard's law.

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Session 9 / **17**

UO2 corrosion by liquid sodium

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In some of the currently developed Sodium Fast Reactor (SFR) designs the core configuration will be rearranged to include internal spent fuel storage positions, with the benefit of avoiding an external sodium pool. However, in-vessel storage of failed fuel pins can lead to a direct contact between coolant and fuel, i.e. in a scenario where the cladding was breached, leading to their potential interaction in case of oxide based fuel forms (UO2 and MOX). The reaction product of sodium and oxide fuel is generally denoted as Na3MO4 (where M=U, Pu), and characterized by unfavorable physical properties, which might result in fuel swelling and/or pulverization, with the consequence of fissile isotopes or fission products dissemination into the primary system. The understanding of the corrosion mechanism and kinetics between liquid sodium and oxide based nuclear fuel becomes then of prior importance for establishing the feasibility of an internal storage of failed fuel pins.
In this contribution, we will present the results of out-of-pile tests that we perform to provide a basic knowledge of defective fuel pin behavior in contact with liquid sodium. With the aim to determine the physical mechanism involved in the sodium-fuel reaction, we firstly focused on the behavior of

UO2 corrosion by sodium.
In order to cover the internal storage scenario, isothermal experiments were performed inside capsules with stagnant liquid sodium and UO2 at 800℃. To establish the influence of the grain orientation on the growth process of the reaction product, well-oriented (<111> and <001>) single crystals were used and finally to extend the behavior to the fuel pellet, a polycrystalline UO2 sample was tested as well. The corrosion product was analyzed by XRD, SEM-EDX and RAMAN. It consists in a homogeneous layer, whose morphology depends on the crystallographic orientation of the UO2 corroded grain or single crystal. However, the thickness of the corrosion layer does not seem to depend on the crystallographic orientation of the UO2 corroded grain that was unexpected.
A tentative interpretation of UO2 corrosion by sodium is proposed. This interpretation will be used for further study on the modelling of MOX-sodium interaction. There the influence of Pu on the corrosion process will be addressed and added to the UO2-Na model.

Session 9 / **45**

Modernization of UO2 nuclear fuel

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The project aims to cover the main aspects of the nuclear industry such as an extension of the fuel campaign and increasing the fuel burn-up depth. The prolongation of nuclear fuel campaign up to 24 months will require uranium-235 enrichment up to ≤5.0%. The nuclear reactor operation at all stages is determined by the reactivity reserve that is expended during its working process. With only one fuel reload per campaign, the energy release profile at the beginning of this campaign will have the maximum unevenness. In the centre of the core, fuel will burn more intensely, and at the edge, it will be slower. To suppress the initial high reactivity in the reactor core, it is necessary to integrate a burnable neutron absorber into a fuel pellet. It should have a high neutron capture cross-section and do not cause the formation of undesirable minor products. Thus, burnable absorbers are needed to control the peak power and regulate the temperature coefficient of reactivity. There are different methods to profile the energy release in the core:
• Integral burnable absorbers ZrB2 to reduce reactivity at the beginning of the operating cycle(s);
• Inert fuel assemblies, which consist of steel or zirconium rods placed in the central part of the core to reduce reactivity.
Successful experience on applying (U, Gd)O2 fuel pellets with ZrB2 coating, deposited onto the surface, provided a higher neutron adsorption abilities for the reactor and resulted in optimizing the economic performance. Comparing characteristics of the UO2 fuel with Gd2O3 and ZrB2 absorbers integrated into it, a greater temperature coefficient of reactivity was observed in the active zone with fuel UO2 + ZrB2. The reason is the difference in the energy dependences of the neutron absorption cross sections: this dependence is more extended in boron. This property of ZrB2 is especially important when increasing the energy intensity of the core and will be crucial for fuel loads designed for more than one year of operation (18 months). ZrB2 is a well-known ultrahigh temperature ceramics finding applications as a burnable absorber. We suggest homogeneous incorporating ZrB2 into the fuel pellet core. Three variants of the fuel pellets were prepared. Wherein, a ceramic pellet of uranium dioxide as standard fuel form was manufactured as an etalon for the further investigations. ZrB2 was integrated in the form of powder and/or micro granules which keeps ZrB2 inside a sealed granule and, hence, requires less amount of absorber per pellet. The concentration of the absorber also plays an important role. As known, an increase in the concentration of Gd2O3 in UO2 fuel to 7% allows for a 12-month duration of the irradiation cycle, the addition of 9wt.% allows to increase the cycle time up to 16 months.
This work is a fundamental stone in developing nuclear fuel manufacturing processes and tackling the challenge of improving the nuclear fuel performance with hybrid fuel assemblies that facilitate longer (24-months). This detailed study constitutes the foundation stone in our understanding the effects of ZrB2 on the fuel performance.

Session 10 / **5**

Peridynamic Modelling of Nuclear Materials

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Peridynamics is a developing non-local modelling technique which has the ability to model crack initiation, propagation and branching. Unlike finite element analysis, the technique uses an integral formulation to determine the forces upon material points. This means that crack patterns can be predicted without any a priori knowledge of the loading or crack pattern. A peridynamic model for nuclear materials is being developed in the Abaqus finite element code. We will address three models which have been developed to date.

SiC/SiC Composite Claddings
Sic/SiC composite claddings are currently being developed as part of a suite of accident tolerant fuels intended as an alternative to the zirconium alloys currently used in light water reactors. Despite their strength and improved oxidation performance, SiC/SiC claddings have a number of drawbacks, namely their irradiation swelling and low thermal conductivity. Their irradiation swelling saturates after a number of months in reactor and is greater on the colder outer surface than the warmer inner surface. This causes a tensile stress on the inside of the cladding. This increases during the decrease in power at the start of a typical pressurised water reactor refuelling outage and causes microcracking of the matrix on the cladding inner surface. In models without fibres, cracks would propagate through the cladding. If fibres are modelled, matrix cracking will extend to a depth of around 20% through the cladding from the inner surface. If an inner monolith of SiC is additionally modelled, cracking propagates through the monolith and acts as a stress raiser for matrix cracking in the composite. If an outer SiC monolith is modelled, fibre pull-out on the inner surface of the cladding was increased by just under 70%.

UO2 Nuclear Fuel Pellets
Nuclear fuel pellets crack duing the initial rise to power in the reactor and subsequent operational changes. This cracking plays an important role in pellet-clad interaction. Our initial work is being extended to take into account the statistical nature of ceramic fracture by carrying the strength of material points.

ZrO2 Cracking and Cladding Oxidation
An zirconia layer forms on nuclear fuel cladding due to the oxidation of the zirconium alloy in the aqueous reactor coolant. The layer is formed with significant anisotropy; the volume gain in the direction of oxide growth being two orders of magnitude greater than that in the direction of oxide growth. Under the stresses induced in the oxide, the oxide cracks. These cracks have been associated with the transformation of the oxidation kinetics from that of parabolic growth of a productive oxide to either breakaway oxidation or repeated transition and parabolic growth.

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Multiscale modelling of cracking in CeO2 and UO2 pellets

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High temperature and temperature gradient in nuclear fuel causes internal stresses in the structure that result fuel deformation, such as swelling, creep and cracking. These phenomena have consequences to e.g. fuel's thermal conductivity and fission gas release, which are critical safety parameters. Currently the modelling of these phenomena mainly rely on empirical correlations. This means

that the models are not extendable to problems beyond the experimental data used in the derivation nor in new fuel designs. More physics oriented and universal solutions can be obtained with decreasing the time and length scales to take into account microscale phenomena and couple them to macroscopic modelling.

We present a comparative study of the cracking in CeO₂ and UO₂ pellets with different centre line temperatures and temperature gradients. In the comparison we apply a multiscale software called properTune [1] developed at VTT and compare the results and modelling to the INL's mesoscale fuel performance code MARMOT [2]. Both codes rely on the MOOSE framework developed at INL. Later on, we plan to compare the results with the corresponding experiments.

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Session 10 / **43**

Development of the 3D Fuel Behaviour Code OFFBEAT

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Several research activities at the LRS of the EPFL and at the PSI aim at developing advanced physics-based and high-fidelity methodologies, in order to improve the understanding of complex phenomena relevant to nuclear reactor safety. In this context, the two institutes are collaboratively developing a new multi-dimensional fuel behavior solver, OpenFOAM Fuel Behaviour Tool (OFFBEAT), based on the open-source C++ library OpenFOAM. The new tool is primarily envisioned as a complement to traditional fuel performance codes and it will be used to investigate the most poorly-known 2D/3D phenomena affecting fuel integrity, such as a missing pellet surface or an asymmetric heat exchange. In this regard, activities are already planned to devise an optimal coupling strategy with the well-known TRANSURANUS code. However, the multi-dimensional feature allows one to use OFFBEAT also for more traditional stand-alone axisymmetric analyses taking into account densification, relocation and swelling strains as well as the temperature and burnup dependence of the material properties with semi-empirical correlations. The development proceeds in parallel with verification and validation efforts. In particular, the contact algorithm and the instantaneous plasticity model for Zircaloy have been verified against available benchmarks and the temperature predictions for axisymmetric rods have been validated against fuel centerline temperature data from the IFPE database. The most recent developments include the introduction of models to take into account the inelastic behavior of Zircaloy, both in terms of instantaneous plasticity and creep, and of the UO2 fuel, with models for fuel cracking and creep. Such models played a fundamental role in the recent 3D analysis of a test-case rodlet undergoing a typical BWR irradiation history in the presence of a missing pellet surface defect. Future works will focus on expanding the 3D study of PCMI to both experimental and full-length rods, including ramp tests and the exchange of information with traditional 1.5D codes. Activities are also planned to use OFFBEAT to interpret the results of UO2 and MOX fuel creep tests characterized by 2D or 3D features, thus assisting the scientific community in the validation of creep models typically used in fuel performance codes.

Session 10 / **29**

Towards improved measurement capabilities and better understanding of the thermo-physical properties of nuclear materials

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The thermo-physical properties of nuclear materials govern the operational and off-normal behavior of a nuclear reactor. It is, thus, necessary to be able to accurately measure and understand these material properties. Frequently, nuclear materials available for examination may be scarce and could come in non-ideal geometries (e.g. fuel fragments or curved cladding specimen). The asymmetry of the sample geometry challenges the accuracy of conventional measurements of thermal diffusivity and conductivity (using techniques as the laser flash method). Hence, in this study the effects of a curved geometry would be examined on the measurements of thermal diffusivity, thermal conductivity and specific heat via the laser flash technique. For this purpose a 3-D finite element model is developed which simulates the heat transfer in a curved Zircalloy cladding segment. The model is used to produce synthetic data which mimics the experimental data obtained during a laser flash experiment. Subsequently, an axisymmetric (2-D cylindrical geometry) model is built approximating the 3-D cladding geometry while conserving volume. The thermal properties (specific heat and thermal conductivity) of the 2-D model are optimized to obtain a minimal least square difference between the 2-D output and the synthetic 3-D data. This has been done over a range of temperatures. Correction factors are established as a function of temperature. Depending on the surface on which 3-D data is calculated (convex or concave) the correction factors differ.

Session 11 / **107**

Dependence of molten salt liquidus temperature on its composition

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Molten Salt Reactors (MSR) are very specific from the fuel properties perspective. Many issues related to the solid fuel behavior are not relevant for this liquid fuel. At the same time, many new issues arise. The viscosity, liquidus temperature, its difference from solidus temperature, thermal conductivity and capacity and many other parameters depends on the fuel composition and its redox conditions.
In this presentation the evolution of liquidus temperature is evaluated for Molten Salt Fast Reactor (MSFR). This reactor uses molten fluorides salt, which roughly consist of eutectic mixture of LiF and AcF4. It is designed for operation in closed Th-U fuel cycle. Nevertheless, it is not so obvious how to reach this state. Basically the are only three available option for initial fuel loading of this reactor: 1) using LWR TRU, 2) using enriched uranium and 3) using mixtrure of both previous options. The transition towards equilibrium Th-U cycle was evaluated for several initial fuel compositions and the evolution of liquidus temperature was observed along each of these trajectories.
The burn up calculations were accomplished by EQL0D procedure using Monte Carlo code Serpent 2 and the liquidus temperature was obtained by GEMS TM core using Heracles database.
During all transitions certain amount of PuF3 was created. Since the solubility of trivalent fluorides in this carrier salts is limited, the respective salt liquidus temperature evolves strongly.
The results of neutronics burn up calculations for each transition paths are presented ins the traditional liquidus temperature diagram. They show the possible range of liquidus temperature and options how to transit towards the equilibrium Th-U cycle.

Session 11 / **104**

The Changing Role of Computation in Material and Process Design

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The presentation starts with a brief review of material design challenges and opportunities presented and discussed in previous NuFuel and MMSNF conferences. It continues with a snapshot of recent results on model development using AI components such as machine learning, computer vision and real-time process optimization. The second part of the talk focuses the knowledge, wisdom and ideas accumulated during the current NuFuel/MMSNF meeting and the emerging topics for future meetings.

Session 11 / **105**

Final discussion

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