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D6.1 Simulation and optimization of performance during normal operating conditions of a minor actinide-bearing fuel pin

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DOCUMENT SUMMARY

Minor actinides are the main contributors to medium- and long-term radiotoxicity and heat production in spent nuclear fuels. Research efforts are currently ongoing to explore different options to dispose of such radionuclides, e.g., their burning and transmutation in fast reactors within mixed-oxide fuels. The MYRRHA sub-critical reactor is one of the future facilities with envisaged burning and transmutation capabilities. This work assesses the thermal-mechanical performance of homogeneous Am-bearing fuel pins both in the In-Pile test Section (IPS) position of the MYRRHA “Revision 1.8” core and under driver irradiation. The normal operating conditions of MYRRHA are considered, with a focus on the safety design limits and involving sensitivity analyses to evaluate the impact of increasing americium contents (in the range 0-5 wt.%) on safety-relevant simulation outcomes. The simulations are performed with the TRANSURANUS fuel performance code coupled with the SCIANTIX physics-based module for inert gas behaviour. They rely on a dedicated surrogate model for the helium source term during MYRRHA irradiation, accounting for the relevant contribution of the fuel americium enrichment, besides advanced models for the properties and behaviour of the specific pin materials. Specifically, models for Am-fuel thermal properties (thermal conductivity, melting temperature, specific heat) developed in Task 5.1 of the PATRICIA Project are used for the simulations. Moreover, high-fidelity boundary conditions (cladding outer temperature, axial coolant pressure) on the MYRRHA pins under IPS irradiation, provided by sub-channel analyses achieved within PATRICIA Task 5.4, are accounted for and their impact showcased on the fuel central temperature as a figure of merit. The analyses reveal the suitability and safety under irradiation of MOX fuels with low Am enrichments according to the current MYRRHA design.

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1 Introduction

Our current society is in the process of transitioning to a more sustainable global system, and while the task ahead is extremely challenging and involves all the human activities, a significant fraction of this effort is related to energy [1]. Nuclear energy can provide a significant contribution to the global effort of phasing out of fossil fuels, but it is still not widely accepted by the population. One of the most recurring themes that hinders nuclear social acceptance is the production and management of long-lived radioactive nuclear waste [2], which is why research on innovative, advanced, and safe methods to dispose this hazardous material is still ongoing [3]–[5]. Indeed, the current fleet of light water reactors produces considerable amounts of high-level waste, and while most of it (U and Pu) can be partially recycled as fuel via e.g., advanced fuel cycle concepts as the twice-through one [6], [7], a fraction of the remaining minor actinides is still a significant contributor to long-term radiotoxicity. The feasibility of the Partitioning and Transmutation (P&T) route for these radionuclides through the use of fast reactors (FR) is being explored [8]–[10]. Advanced FR systems are a sub-set of the Generation IV reactor concepts [11], [12], which comprehends liquid metal-cooled systems featured by an improved sustainability, i.e., a more efficient fuel utilization and minimization of the residual waste from nuclear applications [13], [14].

The PATRICIA (Partitioning And Transmuter Research Initiative in a Collaborative Innovation Action) H2020 Project [15] focuses on developing advanced partitioning techniques to efficiently separate americium from spent fuel and to analyse the behaviour under irradiation of Am-bearing nuclear fuel. In this framework, this work deals with the performance assessment of an Am-MOX pin, i.e., fuelled with (U, Pu, Am)O_{2-x} and designed for transmutation purposes, for future irradiation in the MYRRHA reactor concept [16]. MYRRHA is an experimental FR concept for research applications, cooled by Lead-Bismuth eutectic (LBE) and equipped with an Acceleration Driven System (ADS) coupled to the sub-critical core configuration. Indeed, the MYRRHA reactor, being designed by SCK CEN (Belgium), will have two operating modes: the sub-critical mode and the critical mode. The first one will require a continuous injection of high-energy neutrons, which will be provided via a LINAC (LINear ACcelerator) that is being built at the reactor site. This machine will be capable of accelerating protons up to 600 MeV; these high energies enable spallation reactions on heavy atoms such as the lead and bismuth of the coolant, producing multiple instances of high-energy neutrons. The target of this particle beam will be a channel of liquid LBE located in the centre of the reactor core. This device, in synergy with the LBE coolant, will produce the hardest neutron spectrum ever achieved up to now in a fission reactor. High-energy neutrons are capable to directly split fissionable nuclides, that is why one of the main goals of the MYRRHA facility is to study the P&T of minor actinides, most of them being fissionable nuclides.

The current design specifications of the sub-critical configuration of the MYRRHA reactor ("Revision 1.8", provided within the PATRICIA Project [15]) foresee a thermal power output of 70 MW_{th} produced among 78 fuel assemblies, which will be loaded with a U-Pu MOX fuel encased in a DIN 1.4970 cladding, which is a specific alloy, annealed and cold-worked, of the 15-15Ti stainless steel family. This core configuration is not just composed of fuel assemblies and the central LBE spallation target, but it comprehends some experimental assemblies in the second core ring dedicated to irradiation experiments (IPS - In-Pile test Sections), in which performance testing of Am-MOX pins is envisaged, besides thermal islands for thermal neutron irradiations (ThIPS) and safety rods (CR) in the fourth core ring (Figure 1). Moreover, the core is surrounded by a stainless steel jacket and includes MgO reflector channels and LBE channels at the periphery. The analysis of the IPS irradiation is particularly of interest to understand the behaviour of Am-MOX fuel during a single MYRRHA cycle, to support the qualification of these pins as driver (or blanket) fuel towards advanced configurations of the reactor core devoted to transmutation / burning goals.

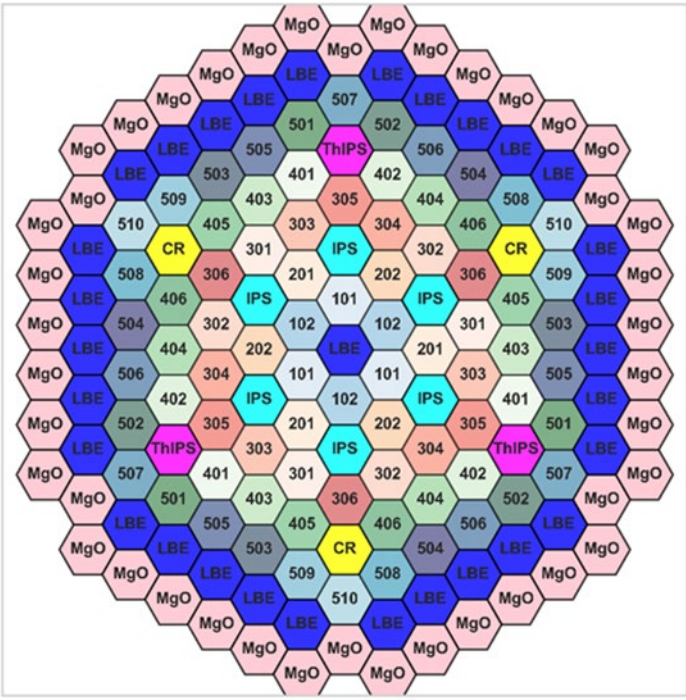

Fig. 1. Scheme of the current MYRRHA "Revision 1.8" core design, sub-critical configuration.

The analyses presented in this work are performed using the TRANSURANUS fuel performance code (FPC) [17], [18], coupled with the SCIANTIX module for inert gas behaviour and release modelling [19]–[22] in support of the design and performance analyses of MYRRHA Am-MOX pins – namely (U, Pu, Am)O_{2-x} fuel with an americium content up to 5% at the IPS location. The focus of this work is on the pin safety under irradiation, determined by comparison with safety limits, as well as on the capabilities of burning americium and on the production of helium in Am-MOX fuels. For this purpose, SCIANTIX has been equipped with a surrogate model for He production dedicated to the MYRRHA fuel composition and irradiation conditions. This model, already reported in PATRICIA Deliverable D5.2 [23] and in [24], is built on synthetic datasets of produced He generated via the burnup module capabilities of SCIANTIX itself [25], [26], fed by neutronic data (cross-sections, besides fission yields and decay constants) derived from a SERPENT modelling and simulation of the MYRRHA pin. Additionally, advanced models for the properties and behaviour of the specific pin materials are used for the simulations, in particular updated models for Am-fuel thermal properties (thermal conductivity, melting temperature, specific heat) developed in Task 5.1 of the PATRICIA Project [27]. The impact of these novel models on the MYRRHA Am-bearing pin performance is showcased in comparison with the use of previous state-of-the-art models from [28]. The impact of high-fidelity boundary conditions (cladding outer temperature, axial coolant pressure) on the MYRRHA pins under IPS irradiation, provided by sub-channel analyses achieved within PATRICIA Task 5.4 [29], is also accounted for and showcased for the IPS irradiation scenario, on the fuel central temperature as a figure of merit. The aim of the Computational Fluid Dynamics (CFD) investigations of the MYRRHA IPS sub-channel was both to obtain reliable thermal-hydraulics boundary conditions for the pin performance, and to develop and demonstrate a methodology to inform pin performance calculations with advanced results from the coolant side. These include e.g., the proper consideration of the coolant velocity, temperature and pressure fields accounting for turbulence effects, besides enabling a better representation of the coolant dynamics during transients compared to empirical correlations (e.g., the Ushakov one [30]) built on data from steady-state experiments.

The deliverable is structured as follows. Section 2 details the specifications of the MYRRHA irradiation scenarios considered in this work, while Section 3 presents the simulation tools and modelling set-up applied to analyse the Am-MOX pin performance. The code results are provided in Section 4 for both the IPS and driver fuel irradiation scenarios, complemented by sensitivity analyses focused in particular on the impact of the fuel composition in terms of Am content. Conclusions are drawn in Section 5, along with suggested further developments following the present work.

2 Specifications of the MYRRHA irradiation scenarios

The focus of the analyses performed in this work is the irradiation in the current MYRRHA "Revision 1.8" core design of a MOX fuel pin loaded with americium, either for 90 days of single-cycle, full power operation within the IPS experimental assembly or as a driver pin experiencing the complete in-reactor history from first loading to discharge at the target burnup. The IPS experiment is indeed mainly designed to qualify Am-MOX pins as MYRRHA driver fuel, i.e., fuel pins irradiated for an extended period of 13 irradiation cycles, each one corresponding to an irradiation position along the MYRRHA core (from the hottest one, in the first core ring closer to the central spallation channel, to the last one in the peripheral fifth core ring). The handling of the fuel assemblies (FAs) follows the reshuffling scheme illustrated in Figure 2a (where the numbers from 1 to 13 correspond to the initial and final positions of the driver FA path during its life in the core) [1] [31]. Each of the irradiation cycles lasts 90 days as the IPS irradiation. The IPS irradiation position is placed in the second ring of the MYRRHA core, just like the second irradiation position for the driver fuel. More specifically, the neutron flux (and consequent linear power produced) that a fuel pin experiences in the IPS is assumed as the average between the two surrounding, second-ring driver positions, i.e., number 201 and 202 (as shown also in Figure 1). For what concerns the thermal boundary condition in the IPS, its primary coolant-cooled configuration is considered in this work (i.e., same LBE inlet temperature and mass flow rate designed for the driver assemblies), while the possibility of an isolated IPS configuration is still under consideration for MYRRHA.

[1] Considering the MYRRHA core symmetry, the driver fuel irradiation is performed in each one-sixth of the core simultaneously. With reference to the core portion highlighted by the red triangle of Figure 2a, the driver fuel irradiation progressively occupies the positions 102 - 202 - 302 - 304 - 306 - 402 - 404 - 406 - 502 - 504 - 506 - 508 – 510.

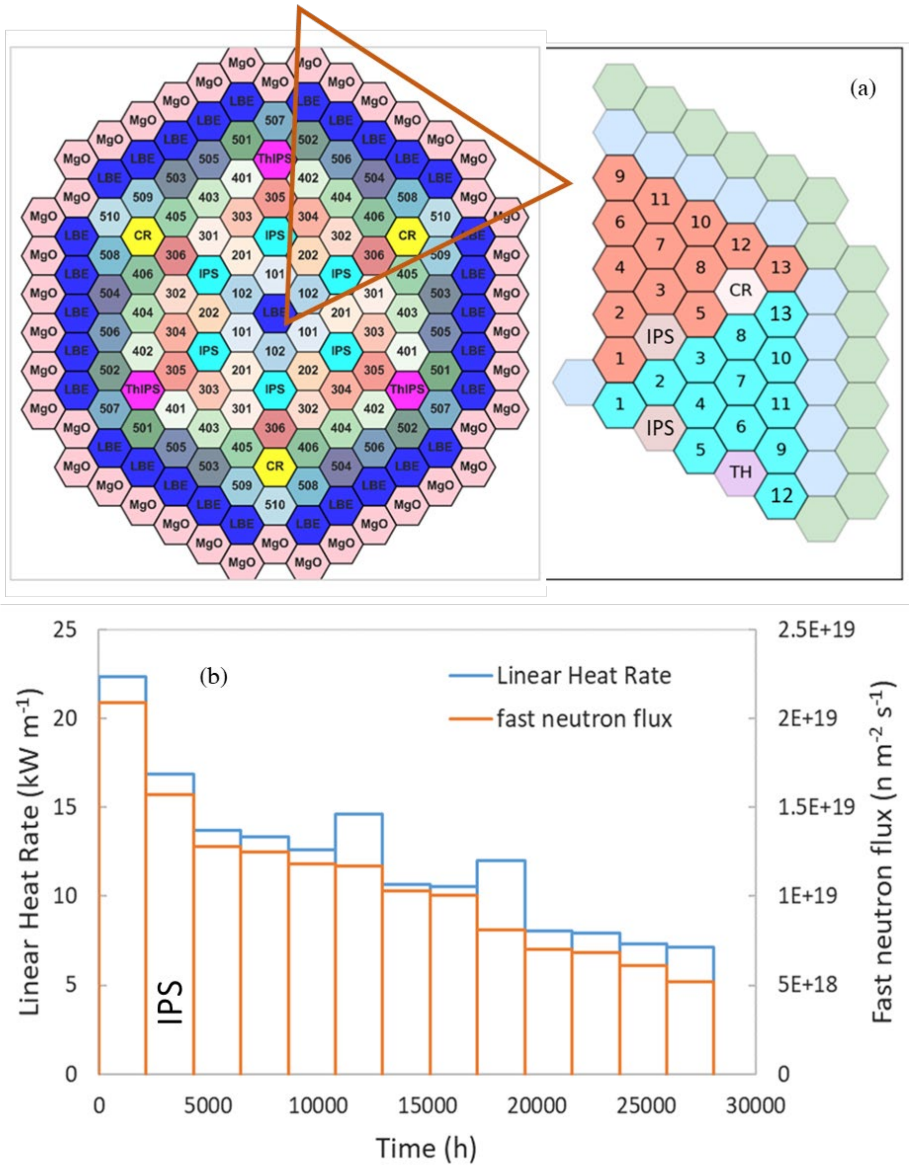

Fig. 2. (a) Scheme of the 13 irradiation positions during the normal operation of the MYRRHA driver fuel [31]. (b) Irradiation conditions of the hottest pin under both IPS and driver scenarios, at the peak power node, corresponding to the specifications of "Revision 1.8" of the MYRRHA reactor core. The values shown correspond to the reference Am-MOX composition designed for MYRRHA, i.e., 0.49 wt.% Am and 29.51 wt.% Pu.

The irradiation conditions shown in Figure 2b correspond to the "hottest" Am-MOX pin, i.e., to the conservative assumption of considering the pin placed in the harshest position (in terms of neutron flux and linear heat rate, and consequently fuel temperature) within the fuel assembly, in each of the irradiation cycles. Hence, the performance of the hottest Am-MOX pin is analysed in this work, according to the same approach already adopted in [31], [32] and applied to MYRRHA U-Pu MOX fuel. This is important considering that a scope of this analysis is to provide indications about the safety of Am-loaded pins under the normal operating conditions designed for the MYRRHA "Revision 1.8" reactor.

For what concerns the fuel composition, the primary option for the current MYRRHA core design foresees an amount of plutonium and americium which correspond together to 30 wt.% of the heavy metals in the Am-MOX fuel. In this study, the homogeneous strategy for the recycling and transmutation of americium is analysed: the reference Am content is set to 0.49 wt.% and the impact of a 5% Am content (limit for the homogeneous strategy for Am recycling) on the pin performance is showcased just under the IPS irradiation. Indeed, the irradiation history (both linear power and fast neutron flux) shown in Figure 2b holds for the reference 0.49 wt.% Am content. The actual neutron fluxes and powers in both the IPS single-cycle and each of the 13 driver irradiation cycles would depend on a different fuel Am content, besides on e.g., the experimental rig and irradiation environment in the IPS position. Therefore, additional neutronic computations for each of the 13 cycles of MYRRHA driver irradiation and specific for each fuel composition (out of the scope of this work) should support the pin performance analyses in case the 5% Am content is considered to fuel driver assemblies. For what concerns the IPS sub-channel, it is specifically designed for experimental irradiation tests of different oxide fuel options (with different Am contents) for MYRRHA. This supports the sensitivity analysis on the fuel Am content performed by considering the IPS irradiation conditions, under the assumption of a negligible impact of Am contents in the range 0.49 – 5 wt.%, assuming that the total heavy metal content in the fuel is unchanged.

For what concerns the main specifications related to core and pin geometries, and as-fabricated material parameters, they are mostly in line with the previous MYRRHA design “Revision 1.6”, already targeted by [31], [32]. They are recalled and collected in Table 1 since MYRRHA “Revision 1.8” is the latest, updated core design targeted by this work and of reference within the PATRICIA Project. The main differences with the previous “Revision 1.6” design consist in the presence of the IPS irradiation position within the second core ring, the Am-bearing mixed-oxide fuel instead of U-Pu MOX, the lower linear heat rates and the lowered coolant inlet temperature (from 245°C to 220°C).

The complete definition of the irradiation conditions for the 13 successive positions of driver fuel irradiation in the reactor core, coherently with Figure 2, is provided in a dedicated file (“Update_MYRRHA_v1.8_subcrit_BOC.xlsx”, prepared by SCK CEN) internal to the PATRICIA Project and available to the Project partners via PATRICIA SharePoint [15]. All the data are related to the “Revision 1.8” of the MYRRHA core design.

Table 1. Geometry specifications of the MYRRHA “Revision 1.8” core and as-fabricated MYRRHA fuel pin.

Parameter	Value
Assembly-level	
Number of fuel pins per assembly	127
Pin pitch (hexagonal lattice)	8.4 mm
Total coolant mass flow rate	71.4 kg s^{-1}
Coolant mass flow rate (pin-centred) [a]	0.48 kg s^{-1}
Coolant passage area (equivalent, pin-centred) [a]	25 mm^2
Coolant inlet temperature	220°C
Coolant inlet pressure	0.6 MPa
Pin-level	
Fuel column length	650 mm
Wire-spacer diameter	1.8 mm
Upper plenum length	60 mm
Lower plenum length	580 mm
Fill gas temperature	20°C
Fill gas pressure	0.1 MPa
Fuel outer diameter	5.42 mm
Cladding inner diameter	5.65 mm
Cladding outer diameter	6.54 mm
Fuel specifications	
Am (reference) concentration	0.49 wt.%
Pu (reference) concentration	29.5 wt.%
U-235 enrichment / U (natural U)	0.711 wt.%
Fuel grain size	10 μm
Fuel oxygen-to-metal ratio	1.969
Fuel density	95% TD
Fuel operation	
Average linear power (IPS)	15.24 kW m^{-1}
Maximum linear power (IPS) [a]	16.87 kW m^{-1}
Average linear power (first cycle)	19.45 kW m^{-1}
Maximum linear power (first cycle) [a]	22.35 kW m^{-1}

[a] The values hold for the hottest pin, supposed to cover “interior” positions within the assemblies (avoiding corner or edge effects), in both the IPS and during each of the 13 cycles of driver fuel operation.

3 Modelling and simulation set-up

The simulation tool employed for the present pin performance analyses is the coupled suite between the TRANSURANUS 1.5D fuel performance code (version v1m4j22) [17], [18], working at the integral scale of the fuel pin for thermal-mechanical evaluations, and the SCIANTIX grain-scale code (originally developed by Pizzocri et al. [19]) devoted to physics-based calculations of inert gas behaviour within the fuel matrix. An advanced version (2.0) of SCIANTIX, object-oriented and with extended modelling capabilities, has been recently developed and assessed [20] and is herein applied.

The modelling set-up employed for the performance analyses of Am-MOX fuels under MYRRHA irradiation scenarios (Section 2) is generally the same as in a recent work targeting the behaviour of U-Pu MOX fuel under MYRRHA transient conditions [32]. In addition to this, a model dedicated to the helium production in MYRRHA Am-MOX, relevant due to the fuel Am content herein considered, is adopted. Moreover, advanced models for thermal properties of homogeneous Am-bearing MOX fuels (U-Pu-Am-O fuel with Am contents < 5%), achieved within PATRICIA Task 5.1 [27], are applied to the MYRRHA scenarios analysed. These models are recalled in the following sub-sections. Besides this, the connection with PATRICIA Task 5.4 is here achieved by additional TRANSURANUS simulations, adopting as input boundary conditions the high-fidelity axial profiles of cladding outer temperature and LBE coolant pressure obtained via OpenFOAM (CFD) modelling and simulation of the MYRRHA IPS sub-channel [29].

3.1 Thermal-mechanical properties and behavioural models

The TRANSURANUS code has been equipped with advanced models of thermal-mechanical properties, suitable for the MYRRHA pin materials (fuel, cladding, coolant) and irradiation conditions, which are here recalled and referenced. First, the models for the thermal properties (thermal conductivity, melting temperature) of Am-bearing oxide fuels proposed and validated in [28] are used as a basis, covering the ranges associated to the MYRRHA irradiation in terms of temperature, Am and Pu contents, deviation from stoichiometry, porosity and burnup (relevant especially for the driver fuel irradiation), and providing explicit dependencies on the fuel Am content. Additionally, the effect of novel, updated models for Am-fuels achieved within PATRICIA Task 5.1 [27] are applied to the MYRRHA scenarios analysed.

Second, recent recommendations for fuel mechanical properties (thermal expansion, elastic moduli), suggested by [33], are employed for the simulations. These models are actually developed for U-Pu MOX, but are still applied in light of the low (homogeneous, within [0 - 5] wt.%) Am concentration in the as-fabricated fuel currently considered for MYRRHA applications. This results in a limited impact on the mechanical properties compared to U-Pu MOX in accordance with [34]–[36] devoted also to thermal properties, hence the models for MOX elastic moduli and strain due to thermal expansion can be deemed suitable also for Am-MOX. This is in line with the state-of-the-art approach for the modelling available in fuel performance codes [37], [38], and the same strategy is adopted for all other fuel properties not mentioned before (e.g., specific heat, creep). For so-called blanket fuel materials, i.e., $(U,Am)O_2$ mixed oxides with higher Am contents (10 – 20%), a dedicated modelling should be necessary to target the effect of such relevant amounts of minor actinides [39].

For what concerns the cladding modelling, the standard TRANSURANUS models for the properties of 15-15Ti steels are adopted, apart from models developed specifically for the MYRRHA cladding steel (DIN 1.4970, of the 15-15Ti steels family) and published in [31]. These models concern the thermal and irradiation-induced creep, void swelling and time-to-rupture, applicable to ranges relevant for the current MYRRHA core design. Advanced models are also implemented in TRANSURANUS and employed for the thermo-physical properties of the LBE coolant (e.g., thermal conductivity, specific heat, viscosity), aligned with the recommendations provided by the latest NEA Handbook [40]. The heat transfer coefficient between cladding and coolant is modelled via the Ushakov correlation [30], of reference in TRANSURANUS for lead / bismuth / LBE coolants. Additional correlations suitable for LBE (i.e., those by Subbotin and Kazimi-Carelli, reviewed by [41] and recently by [42]) prove to be more conservative in the MYRRHA normal operation conditions since providing a lower Nusselt number (~ 20-25% lower). This range corresponds to the variation of the LBE Nusselt number considered in the sensitivity analysis performed in Section 4.3. The TRANSURANUS simulations reported in this Deliverable are also informed by high-fidelity thermal-hydraulic boundary conditions (axial profiles of cladding outer temperature and LBE coolant pressure) from OpenFOAM modelling and simulation of the MYRRHA IPS sub-channel [29]. The associated effect on the fuel central temperature, as a most relevant pin performance figure of merit, is showcased in Section 4.1.

3.2 Inert gas behaviour modelling

The most important advancement concerning behavioural models consists in the use of SCIANTIX (version 2.0 [20]) as a physics-based module dedicated to inert gas (xenon, krypton, and helium) behaviour coupled to TRANSURANUS. This enables a coherent calculation of fuel swelling and gas release [2] in the fuel-cladding gap resulting from the intra- and inter-granular description of the gas dynamics accounting for lower-length scale data and information embedded in the model parameters (e.g., diffusivities, trapping and re-solution rates, fractional coverage of the grain boundaries) [20], [43], [44]. In this way, the FPC benefits from the bridging with the atomistic scale according to a consistent multi-scale framework, and overcomes the correlation-based modelling typically adopted by engineering software. The physics-based nature of the SCIANTIX modelling, with parameters adjustable to account for specificities of different types of oxide fuels, guarantees the general validity and applicability of the model also to the Am-bearing oxide fuels designed for MYRRHA. Moreover, applying a mechanistic inert gas behaviour modelling is relevant to target peculiar irradiation conditions as the MYRRHA ones (low pin linear power compared to typical FR designs), resulting in a better representation of the higher gas retention and associated fuel gaseous swelling.

When running the TRANSURANUS//SCIANTIX coupled code suite, SCIANTIX is called by TRANSURANUS at every radial/axial node of the adopted fuel discretization mesh, within each calculation loop that the FPC performs at each time step. This happens online during the simulation, according to a coupling methodology and interface developed in [21], [45]. The coupling between TRANSURANUS and SCIANTIX is already demonstrated and assessed in previous works from the same authors, concerning the application of the coupled suite to both water-cooled and liquid metal-cooled irradiation experiments and reactor designs [22], [32], [38], [46]–[48]

As part of a dedicated modelling of helium behaviour in Am-bearing fuels, the TRANSURANUS//SCIANTIX coupled suite is equipped with a surrogate model for He production in Am-MOX under MYRRHA irradiation conditions. This is derived from a SERPENT neutronic modelling of the MYRRHA Am-bearing pin, providing cross-sections customized for the MYRRHA reactor, and from subsequent runs of the SCIANTIX burnup module capabilities to generate high-fidelity estimations of He produced in ranges of fuel composition and irradiation conditions relevant to the current MYRRHA

[2] The release of both helium and fission gases from the fuel grain boundaries to the pin free volume, during the coupled TRANSURANUS//SCIANTIX simulation, is handled by SCIANTIX based on the evaluation of the fractional coverage of the grain boundaries by inter-granular bubbles. When this fractional coverage overcomes a grain boundary saturation threshold, the excess gas is released so that the equilibrium condition is restored [20], [55].

design. The remarkable agreement between the predictions provided by SCIANTIX and the high-fidelity values from SERPENT represent the verification of the SCIANTIX calculations and result in an advanced and more reliable estimation of the He produced especially at higher Am enrichments, compared to standard burnup modules generally employed by fuel performance codes [24]. The artificial He production data generated via SCIANTIX are best-fitted and assessed to derive a surrogate model dedicated to the current MYRRHA design, with the aim to describe He production accounting for the actual conditions and fuel composition (especially in terms of Am) during the MYRRHA irradiation. Additionally, a surrogate model allows faster computing times, suitable for implementation in / coupling with fuel performance codes, compared to the running times of burnup modules [25]. Complete details about this MYRRHA-oriented model, used for the simulation results presented in what follows, are provided in [24].

4 Fuel pin performance results

The results of the MYRRHA Am-MOX pin performance are provided and discussed in this Section, obtained by calculations performed as indicated in Section 3 (including the dedicated model for He production) and with reference to the core configuration, specifications and scenarios introduced in Section 2. The analysis focuses on two different fuel compositions of interest in terms of americium content, i.e., 0.49 wt.% which is considered as the reference for the current MYRRHA design (hence 29.5 wt.% Pu), and 5 wt.% Am (25 wt.% Pu) as it represents the upper limit for the homogeneous Am composition. The aim is to analyse the sensitivity of pin performance figures of merit to the fuel Am content, providing indications on the possibility to load the MYRRHA fuel with more Am than in the reference as-fabricated pellets. It is worth noticing that different fuel compositions, hence different Am contents, surely correspond to different local power and fluxes at both IPS and driver irradiation positions. For this reason, the sensitivity to the fuel Am content of pin performance figures of merit is showcased in the IPS scenario, designed for this kind of experimental irradiations and studies and under the assumption that Am contents in the range [0 - 5] wt.% do not significantly impact on the IPS irradiation conditions (Figure 2b, referred to the 0.49 wt.% Am content and currently available via the PATRICIA Project [15]). Instead, the behaviour under driver irradiation of MYRRHA Am-pins is studied for the reference Am composition (0.49 wt.%, corresponding to 29.51 wt.% Pu), for which the irradiation conditions are currently and strictly provided.

First, simulation outcomes related to safety limits imposed on the pins in the current MYRRHA design are illustrated in Section 4.1. Then, Section 4.2 provides insights on the inert gas behaviour accounting for the impact of different Am contents, while an extended sensitivity analysis involving additional key parameters / models for the pin thermal-mechanical performance is provided in Section 4.3.

4.1 Safety figures of merit

It is fundamental to focus first on the pin safety under irradiation to ensure that relevant operational values, as provided by fuel performance code computations, never reach the safety limits set for MYRRHA [31], both under IPS and driver irradiation. One safety limit is set on the peak fuel temperature, whose maximum value must be lower than the conservative value of 2600°C during any reactor operative condition [31] to avoid any issue related to incipient fuel melting. Figure 3 – left shows the wide safety margin respected by MYRRHA pins loaded with Am-MOX fuel at the reference Am composition (0.49 wt.%), since the maximum fuel temperature overall reaches ~ 1450°C both during cycle 1 (when the pin maximum linear power occurs, i.e., 22.35 kW m^{-1}) and cycle 6 (when the power increases at ~ 15 kW m^{-1} and the burnup effect on the fuel thermal conductivity plays a significant role [28], besides an already significant fission gas release degrading the gap conductance). If the IPS scenario is considered, with fresh fuel introduced in the experimental rig within the second MYRRHA core ring for a single-cycle irradiation at 16.87 kW m^{-1} (peak power), the maximum fuel temperature is limited to ~ 1110°C just after the start-up power rise, when the fuel-cladding gap is the widest and hence gap conductance the lowest.

If the 5 wt.% Am content in the as-fabricated fuel is considered, its impact on the fuel central temperature at beginning of irradiation conditions in the IPS sub-channel is indicated in Figure 3 – right. An increased Am concentration has a negative impact on the margin to fuel melting since the predicted fuel temperatures increase due to the lower thermal conductivity of Am-MOX fuel compared to U-Pu MOX [28], [49]. Additionally, the melting (solidus) temperature of oxide fuel is degraded by the Am content, but still higher than the conservative safety limit set at 2600°C [28]. For the 5 wt.% Am-MOX fuel, the maximum temperature during IPS irradiation increases up to almost 1200°C. Hence, it still never gets close to the limit value against fuel incipient melting issues, confirming the safety under irradiation of MYRRHA Am-MOX fuels, as already demonstrated for U-Pu MOX fuel [31].

Figure 3 – left showcases the effect of the updated modelling of Am-MOX thermal conductivity [27] on the fuel central temperature, compared to the use of state-of-the-art models from [28]. Differences emerge in particular during driver irradiation, due to a different (stronger) degradation of the thermal conductivity according to the novel model. As a consequence, the predicted peak fuel temperature becomes 1495°C, reached during the sixth irradiation cycle. Instead, the use of high-fidelity pin boundary conditions from OpenFOAM [29] does not lead to significant differences under MYRRHA normal operating conditions, as indicated by the red curves of Figure 3 -right, referring to both the 0.49% and 5% Am loading cases. Table 2 collects the results of maximum fuel temperature and associated margin to safety limit at the beginning of IPS irradiation, coherently with Figure 3 – right, representative of the effect of different Am contents on safety-relevant simulation outcomes.

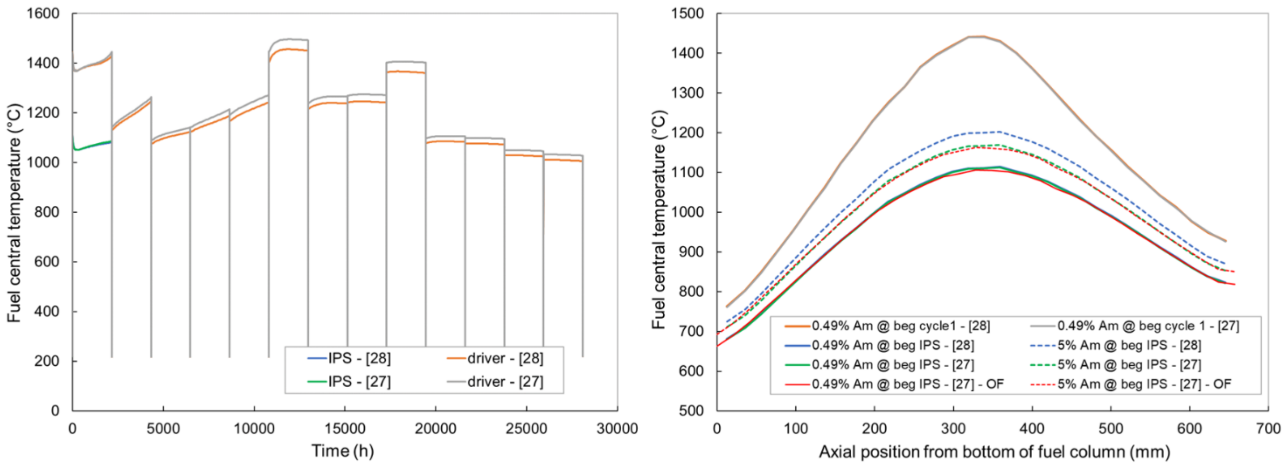

Fig. 3. Left: Evolution of the fuel central temperature at the peak power node during the MYRRHA IPS and driver irradiation, for the reference Am content (0.49 wt.%). Right: Axial profiles of fuel central temperature at beginning of irradiation in the two scenarios, for two different fuel Am contents (0.49 wt.% - reference and 5 wt.%). Results associated to state-of-the art [28] or updated [27] models for fuel thermal properties are presented, together with results from simulations informed by OpenFOAM boundary conditions (OF [29]).

Table 2. Results for the fuel central temperature and margin to safety limit (2600°C) at beginning of IPS irradiation, associated to the simulation cases investigated in Figure 3 - right: state-of-the art [28] or updated [27] models for fuel thermal properties, information on pin thermal-hydraulic boundary conditions from OpenFOAM (OF [29]). The considered melting temperature models provide values higher than the safety limit (2600°C): 2733.0°C / 2734.6°C for 0.49% / 5% Am, from [28]; 2771.0°C / 2776.9°C for 0.49% / 5% Am, from [27].

Simulation case	**Fuel central temperature (°C)**	**Margin to safety limit (°C)**
0.49% Am - [28]	1114.1	1485.9
5% Am - [28]	1203.0	1397.0
0.49% Am - [27]	1112.7	1487.3
5% Am - [27]	1169.4	1430.6
0.49% Am - [27] - OF	1106.0	1494.0
5% Am - [27] - OF	1163.2	1436.8

A second safety limit concerns the plastic strain of the cladding, which is allowed up to 0.5% [31]. Plasticity is avoided if the material behaviour remains within the elastic regime, i.e., the equivalent stress is below the yielding stress, which can be conservatively estimated at around 400 MPa for DIN 1.4970 under the worst MYRRHA conditions in terms of cladding temperature [31], [32]. No fuel-cladding mechanical interaction (gap closure) is observed from the simulations performed of Am-MOX pins under MYRRHA normal operating conditions (Figures 4 and 5 showing that the pellet-clad gap always remains open), so the only contributors to the cladding stress state are the pressure loadings on the cladding (from the gas in the gap on the inner surface, while from the coolant on the outer side), and the thermal gradient across the cladding causing thermal stresses. Moreover, especially during IPS irradiation, the cladding is not subjected to relevant deformation gradients potentially inducing higher stresses, since e.g., the incubation threshold for the void swelling of the cladding is not effectively reached. This results in limited values of von Mises equivalent stress in the cladding during both IPS and driver irradiations, i.e., the maximum values are ~ 53 MPa at the beginning of the IPS cycle and ~ 69 MPa at the beginning of the driver irradiation, both at the cladding inner surface and independently of the fuel Am content. These values are well below the cladding yield stress under any MYRRHA condition and consequently below the safety limit preventing the cladding plasticity. For what concerns the cladding deformations during irradiation, according to their modelling specific for the DIN 1.4970 cladding steel [31], [50], [51], irradiation-induced creep is dominant during IPS irradiation, while cumulative void swelling enters into play together with irradiation-induced creep during driver irradiation, by reaching the incubation threshold for void swelling to effectively start. Instead, thermal creep does not play a significant role in the behaviour of the MYRRHA cladding, considering the limited temperature and temperature gradients across the cladding (at every axial location). These considerations hold also if the updated models for fuel thermal properties [27] or the high-fidelity boundary conditions from OpenFOAM [29] are considered, since the fuel behaviour (slightly different) does not impact on the cladding (no fuel-cladding interaction under open gap conditions) and the updated boundary conditions on the outer cladding provide pin-level results still in line with the TRANSURANUS//SCIANTIX simulations relying on the TRANSURANUS thermal-hydraulic model.

Figures 4 and 5 provide the evolution of fuel-cladding gap width, which remains always open even at the end of the 13-cycles driver irradiation scenario, hence no concerns arise about fuel-cladding mechanical or chemical interaction (which can potentially result in cladding inner corrosion at gap closed). The gap progressively reduces under irradiation at every pin axial location, as driven by the differential radial deformations of fuel and cladding, caused by thermal expansion, creep and swelling, and dominated by the fuel (hotter than the cladding). The minimum gap width occurs at the end of cycle 13 just before reactor shutdown, and corresponds to ~ 40 µm for the pin loaded with 0.49 wt.% Am-MOX. A narrower gap during IPS irradiation is associated to the 5 wt.% Am-MOX case (Figure 4 – right), explained by a hotter fuel resulting in higher thermal expansion and temperature-driven deformations. If the 5% Am fuel would be subjected to driver irradiation, a thermal feedback by a significantly higher helium production and release compared to the reference fuel composition is expected. A substantial amount of He in the gap has a beneficial effect on the gap conductance (compared to a gap composition dominated by gaseous fission products – Xe and Kr), hence the temperature regime in the fuel should become slightly lower, which limits the fuel deformation mechanisms and contributes to keep the gap wider. The use of updated material properties (fuel thermal conductivity in particular) [27] results in slightly wider fuel-cladding gaps at beginning of irradiation conditions, in line with slightly lower fuel temperatures (Figure 3 – right). This effect is more visible for the 5% Am fuel case, for which the novel thermal conductivity model provides higher values compared to the state-of-the-art model [28] for the same composition, before irradiation effects (stronger according to the novel model) come into play.

Given the LBE cooling environment, a safety limit is also set to prevent external cladding corrosion from the coolant, i.e., the coolant temperature must never exceed 400°C, according to a lowered (conservative) safety threshold for MYRRHA "Revision 1.8" to further increase the safety margins during operation. Moreover, a lower inlet coolant temperature is currently adopted (i.e., 220°C compared to 245°C in MYRRHA "Revision 1.6" [31], [32], [52]), together with a lower pin power (16.87 kW m^{-1} compared to 19.5 kW m^{-1}, in the second ring where the IPS is located). As shown in Figure 6 - left, the IPS scenario is clearly within these limits along the entire pin axis (independently of the fuel Am content), with the coolant maximum (outlet) temperature of about 350°C and the cladding outer temperature reaching 362°C at the top of the fuel column after an irradiation cycle under IPS conditions. At the first cycle of the driver irradiation (within the first core ring, the closest to the central spallation channel, and hence at the highest MYRRHA power), the safety threshold is still respected with a lower margin. The coolant outlet temperature is around 380°C and the cladding outer temperature reaches 395°C at the top of the pin (Figure 6 – right), values still limiting the concerns about cladding outer corrosion [3].

[3] The oxidation of the cladding outer surface caused by the corrosive action of the LBE coolant is not considered by the simulations presented in this work, due the current lack (generally in literature and in the TRANSURANUS code) of a corrosion model specific to the couple DIN 1.4970 cladding – LBE coolant and to the MYRRHA conditions. This is recognized as a relevant future development, and a dedicated model will be implemented in TRANSURANUS and tested on MYRRHA as soon as it will be available. Additional effects impacting on the cladding temperature (and hence on the corrosion dynamics) are local hotspots due to the wire spacers, and the boundary layer associated to the LBE coolant. These are out of the modelling capabilities of the TRANSURANUS fuel performance code, but can be accounted for by an advanced modelling of the coolant sub-channel via high-fidelity thermal-hydraulics codes / capabilities, e.g., via OpenFOAM (as already demonstrated in PATRICIA Deliverable D5.4 [29]).

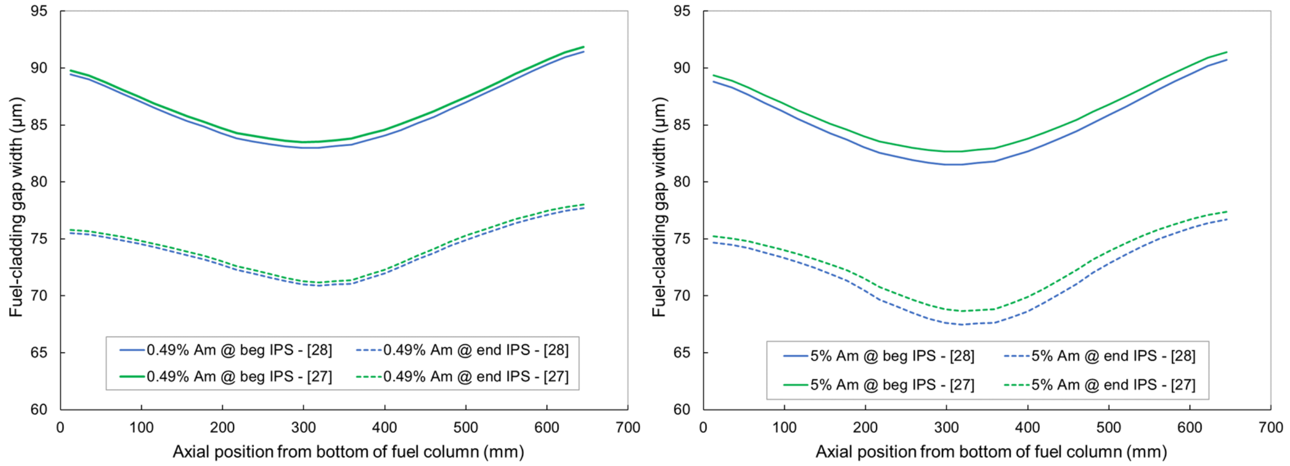

Fig. 4. Axial profiles of fuel-cladding gap width during the MYRRHA IPS irradiation, for two different fuel Am contents: 0.49 wt.% - reference (left) and 5 wt.% (right). Results associated to state-of-the art [28] or updated [27] models for fuel thermal properties are presented.

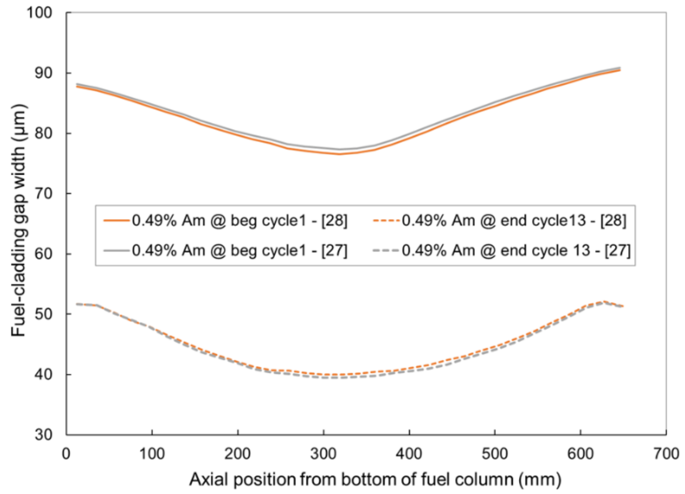

Fig. 5. Axial profiles of fuel-cladding gap width during the MYRRHA driver irradiation, for the reference as-fabricated fuel Am contents (0.49 wt.%). Results associated to state-of-the art [28] or updated [27] models for fuel thermal properties are presented.

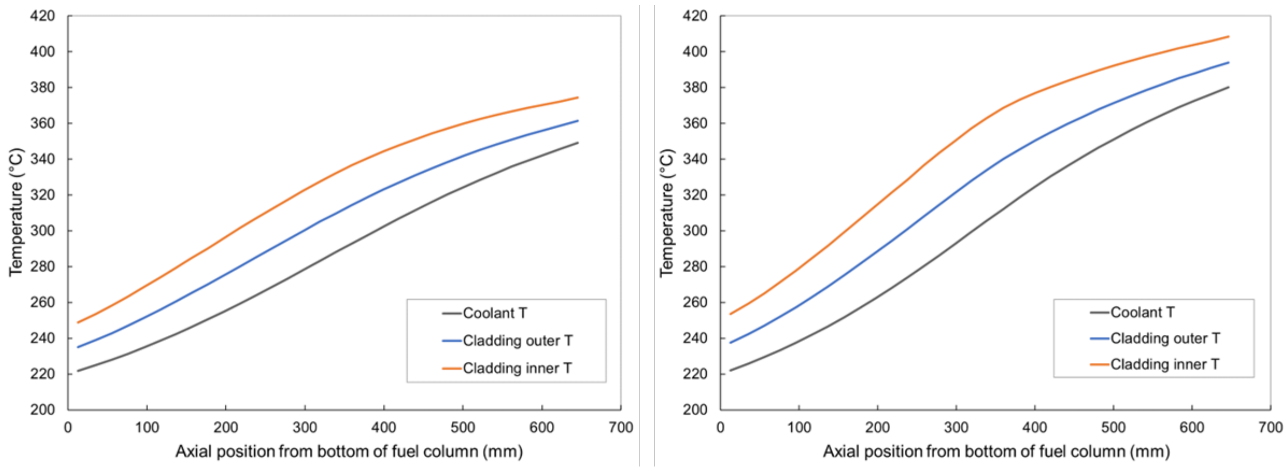

Fig. 6. Axial profiles of coolant temperature, cladding outer and inner temperatures during the MYRRHA IPS irradiation cycle (left) and of the first cycle of the driver irradiation (right).

4.2 Inert gas behaviour

The behaviour of inert gases (fission gases – xenon and krypton, and helium) within the fuel is relevant to the pin performance assessment since it impacts the thermal conductance of the fuel-cladding gap via gas release from the fuel, and the fuel swelling coherently. Moreover, the gas retained in the fuel contributes to the degradation of fuel thermal-mechanical properties (e.g., thermal conductivity), while the gas release determines the gap pressurization and hence the mechanical stress levels in the cladding.

The SCIANTIX grain-scale code, coupled to TRANSURANUS as an inert gas behaviour module [20]–[22], [32], [45] (Section 3), allows a physics-based description of gas behaviour in the fuel leading to coherent evaluations of fission gas release and gaseous swelling. The coupling hence enables the evaluation of integral effects of gas-related dynamics, including helium and its production in MYRRHA Am-oxide fuels according to the specific model applicable to both the IPS and driver irradiation scenarios [23], [24]. This surrogate model represents explicitly the He production by Am-241 and also, in an engineering way via the irradiation time variable, the contribution to He production of nuclides that are produced via neutron absorption on Am-241, e.g., Cm-242 and Pu-238 which are strong α-emitters as well. For this reason, if different axial locations along the fuel stack are considered, He production is enhanced at the peak power node where the neutron flux is maximum.

The novel model tailored for MYRRHA Am-MOX [23], [24] provides a higher helium source term compared to that predicted by the standard burnup module embedded in the TRANSURANUS code (TUBRNP [53], [54]), already in the IPS irradiation case (Figure 7 - left) with even larger differences during prolonged irradiations (driver scenario). This effect is visible especially at 5 wt.% initial Am content in the fuel, while for the reference 0.49 wt.% Am content the He production predicted by the surrogate model or by TUBRNP is similar. The differences between the predictions of the surrogate model for MYRRHA and TUBRNP are linked to the extensive consideration of α-decaying actinides, besides other factors discussed in [25]. Nevertheless, even at 5 wt.% Am content, the integral effects on the overall pin performance during the IPS irradiation are limited, e.g., concerning the evolution of the gas pressure in the pin free volume (Figure 7 – right). Indeed, the gas diffusion phenomena and gas bubble dynamics that occur within the fuel, where inert gases are produced, are heavily influenced by the working temperatures, i.e., the higher the temperature, the faster the inert gases diffuse to the grain boundaries, where they accumulate and will eventually be released into the pin free volumes (gap, plenum) [20]. The relatively low temperatures experienced by the fuel in the current MYRRHA design (Figure 3) and the short duration of the IPS irradiation determine that a negligible amount of inert gases is released in the gap, as indicated by the slight gap pressure increase up to less than 0.2 MPa at the end of the IPS single-cycle. Increasing the fuel Am content corresponds to a hotter fuel, hence to an enhanced diffusion of gas to the grain boundaries and consequent gas release as a result of the inter-granular gas dynamics modelled in SCIANTIX [19], [20], [55].

Figure 8 - left shows the production and release of inert gases during the entire driver irradiation, for the reference 0.49 wt.% fuel Am content. Driven by both fission gas and helium release, the gap pressure continuously increases up to ~ 1.6 MPa at the end of the driver irradiation (Figure 8 - right). Nevertheless, as already explained in Section 4.1, even at the end of the pin life in MYRRHA, the safety limit on the cladding plasticity is not challenged, and the pin performance keeps safe from both the mechanical and thermal points of view. During the single-cycle IPS irradiation, the gas release in the pin free volume is not significant, and consequently the pin inner pressure increase is limited, as already shown by Figure 7 - right. The duration of the single-cycle IPS irradiation is too short for reaching the saturation threshold for gas retention, which is the main reason for a limited gas release. Instead, during the 13 cycles of driver irradiation the saturation is reached after around 2000 hours, then the gas release is enabled and evolves up to a fractional release of around 50% for the fission

gases, and 70% for He. The application of the novel model for Am-bearing fuel thermal conductivity [27] provides a (slight) increase of both fission gas and helium release, due to slightly higher fuel temperatures during driver irradiation determined by a stronger degradation of the property with burnup compared to the state-of-the-art model [28]. An enhanced helium production and release is expected from the simulation of 5 wt.% Am fuel under driver irradiation [24], contributing to both fuel swelling from helium retention and gap pressure increase from a substantial helium release, with beneficial effects on the gap conductance.

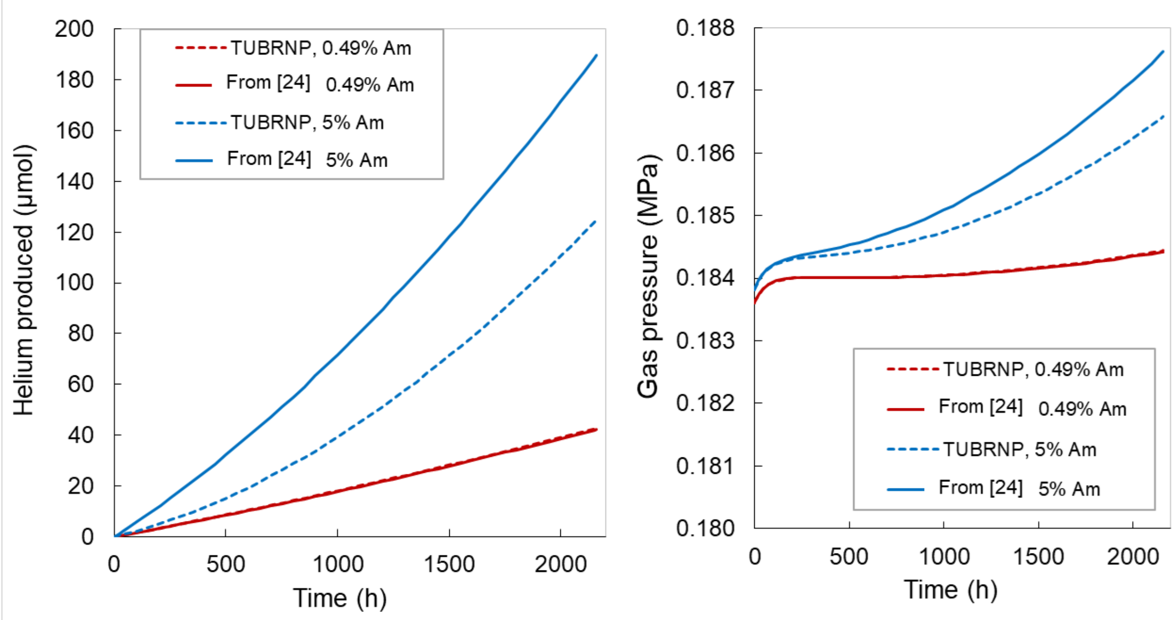

Fig. 7. Evolution of helium production (left) and gas pressure (right) during the MYRRHA IPS irradiation, for two different fuel Am contents (0.49 wt.% - reference and 5 wt.%). The results obtained with the standard TRANSURANUS code (TUBRNP burnup module) are compared with those from TRANSURANUS//SCIANTIX equipped with the He production model for MYRRHA Am-MOX fuels [23], [24].

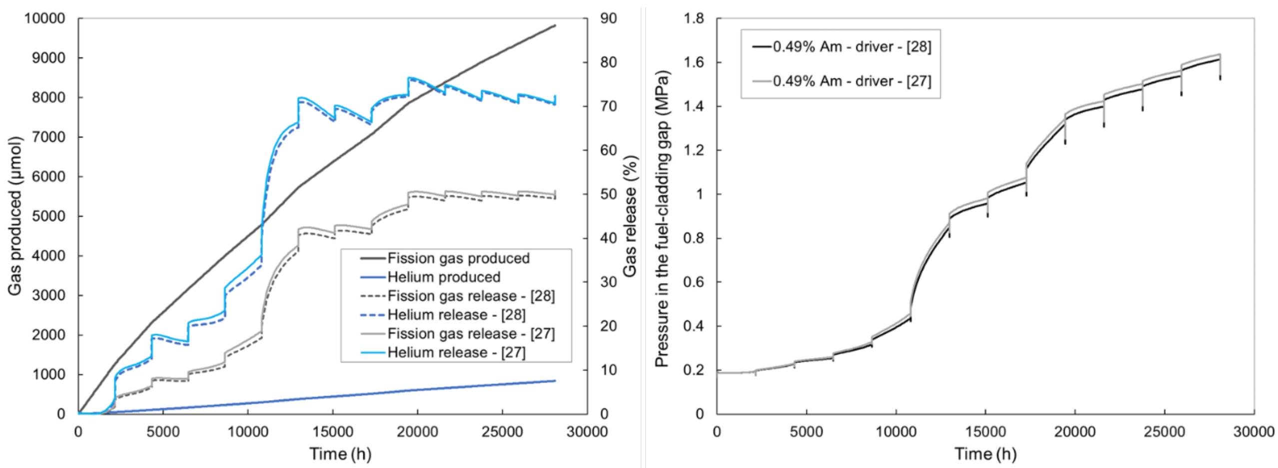

Fig. 8. Left: Evolution of the production and release of inert gases during the MYRRHA driver irradiation of Am-MOX fuel, for the reference as-fabricated Am content (0.49 wt.%). Right: Evolution of the pressure in the pin free volume during the MYRRHA driver irradiation of Am-MOX fuel, for the reference as-fabricated Am content (0.49 wt.%). Results associated to state-of-the art [28] or updated [27] models for fuel thermal properties are presented.

4.3 Sensitivity analysis on safety parameters

The fuel americium content is not the only parameter that can impact on safety-relevant figures of merit. There are multiple other factors that must be considered, some of which come with significant uncertainties. Hence, a sensitivity study is performed via a Pareto analysis [56]–[58] to assess how significant is the impact of the as-fabricated fuel Am loading (within the homogeneous concentration range [0 - 5] wt.%) on safety-related simulation results, compared to that of other variables accounting for their intrinsic uncertainties. Uncertainty is intended here both as the modelling one, linked to the choice of different models for the same phenomenon or property, and the experimental one associated to the available measurements of a certain property or parameter. The properties / phenomena considered and the associated ranges of values or models explored are collected in Table 3. The sensitivity analysis is applied here to the single-cycle IPS irradiation, by referring to state-of-the-art models for fuel thermal properties and pin boundary conditions in line with [24], to draw first but meaningful MYRRHA-oriented indications extendable to additional modelling choices or to the complete driver fuel irradiation. This is supported by the limited impact reported here, for the MYRRHA scenarios analysed, of updated property models [27] or high-fidelity thermal-hydraulic boundary conditions from [29]. Moreover, the single-cycle IPS irradiation is the case study enabling the sensitivity analysis to the Am content.

As already stated in Section 4.1, the margin to fuel melting is a fundamental safety figure of merit that must comply with a safety limit during any operative irradiation condition (both normal operation and transient scenarios). As shown by Figure 9, it is mostly influenced by the choice between different models of the gap conductance [59], [60], while the impact of different initial Am concentrations between 0 and 5 wt.% in the fuel [4] is lower and comparable to that attributed to the uncertainty on fuel thermal conductivity [28] or to the activation of the coupling with SCIANTIX for the physics-based inert gas behaviour [20] (already applied to fast reactor cases [38], [48], and to MYRRHA in [32]).

[4] The fuel Am content impacts on safety-relevant figures of merit not just via the fuel composition (different enrichment levels), but also via its effect on fuel properties, e.g., thermal properties such as the thermal conductivity and melting temperature, fundamental for the margin to fuel melting. A deep analysis of their dependencies on the Am content is presented in [28] (providing the recent models for thermal properties of Am-MOX employed in this work - Section 3.1) and in previous literature works cited therein. Americium is identified as a relevant contributor to the degradation of the fuel thermal conductivity, together with the temperature and irradiation effects, while its impact on the melting temperature is small compared to that associated to deviation from fuel stoichiometry (oxygen-to-metal ratio) and burnup.

Table 3. List of parameters / phenomena involved in the sensitivity analysis to assess their impact on safety figures of merit, by considering the associated modelling / experimental / design uncertainties [5].

Parameter / Phenomenon	**Models / uncertainty**
Fuel Am content	[0 - 5] wt.%
Gap conductance	Models available in TRANSURANUS [59], [60] ± 30% [59], [61], [62]
Fuel densification	FBR models available in TRANSURANUS [63], [64]
Fuel thermal conductivity	± 20% [28], [49]
Linear power	± 5%
LBE Nusselt number	± 25% [41], [42]
LBE inlet temperature	± 10°C
SCIANTIX coupling	On / off

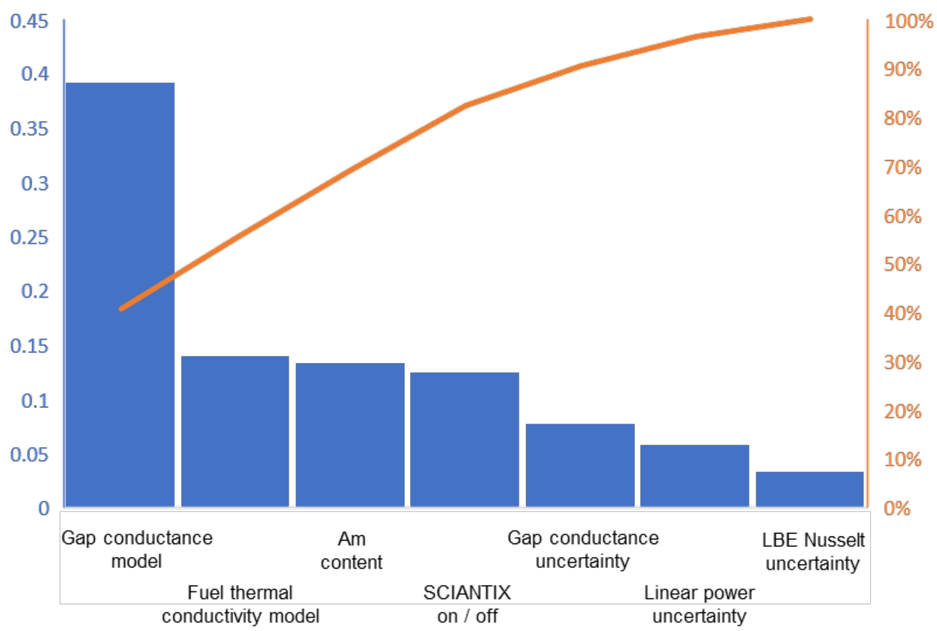

Fig. 9. Pareto diagram showing the sensitivity of the margin to fuel melting to different parameters or phenomena, according to their current modelling in TRANSURANUS//SCIANTIX and to the associated uncertainties.

[5] The parameters / phenomena involved in the sensitivity analysis are relevant for their (direct) impact on the compliance with the safety limits currently set for MYRRHA. Specifically, the linear power, the LBE Nusselt number and LBE inlet temperature determine the cladding temperature (corrosion), while the fuel Am content, the gap conductance modelling, fuel densification and thermal conductivity impact the fuel central temperature (margin to fuel melting). The treatment of the inert gas behaviour and release, linked to the coupling of TRANSURANUS with SCIANTIX, provides the mechanical loading on the cladding (open gap condition) and consequently the cladding stress state. The uncertainties involved are assumed based on literature indications (referenced in Table 3) or are suggested by the MYRRHA design team (within the PATRICIA Project) for what concerns the fuel Am content, the related pin linear power, and the inlet temperature of the LBE coolant.

Figure 10 - left shows that the fuel Am content in the range [0 - 5] wt.% has a limited (indirect) effect on the gas pressure in the pin and hence on the cladding stress levels when the gap is open, via the Am role on the production of helium, whose dynamics and release is considered by SCIANTIX, and on the fuel thermal conductivity. Specifically, the gas release in the fuel-cladding gap is slightly impacted by the fuel Am loading since it influences the fuel temperature regime driving the gas diffusion within the fuel matrix. Nevertheless, the Am effect on the gas pressure in the pin is obscured by other parameters and phenomena strongly acting on the fuel temperature, i.e., the thermal boundary condition provided by the external LBE coolant (in terms of both inlet temperature and heat transfer coefficient between cladding and coolant) and the gap conductance. Section 4.2 already illustrated the limited over-pressurization of the 5 wt.% Am-MOX pin compared to the 0.49 wt.% one, under both IPS and driver irradiation scenarios.

Moreover, Figure 10 – right confirms that the fuel Am content has no effect on the inner / outer cladding temperatures (crucial to prevent cladding corrosion), as anticipated in Section 4.1. This is expected since the cladding thermal performance is dominated by the inlet temperature of the coolant and by its heat transfer coefficient with the cladding.

Thus, it can be concluded that the only safety figure of merit that is significantly influenced by the initial americium content in the fuel is the margin to fuel melting, mainly because of the effect that americium has on both thermal conductivity and melting temperature of oxide nuclear fuels [28] and on the gap conductance via helium release as discussed in Section 4.2.

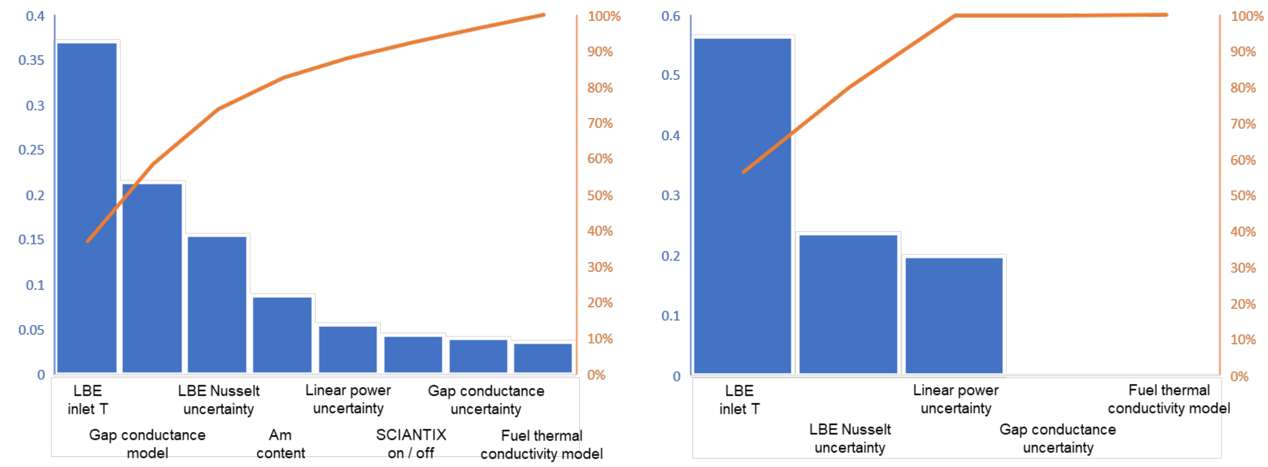

Fig. 10. Pareto diagrams showing the sensitivity of the gas pressure in the pin (left) and cladding outer temperature (right) to different parameters or phenomena, according to their current modelling in TRANSURANUS//SCIANTIX and to the associated uncertainties.

5 Conclusions and further developments

The current design of the MYRRHA sub-critical reactor ("Revision 1.8") is equipped to host Am-MOX experimental fuel pins for irradiation experiments and safety studies, and the pin performance analyses performed in this work confirm that the use of such fuel as a MYRRHA driver fuel is a feasible and safe option since the pin behaviour under irradiation keeps widely within the safety limits. This work hence supports an extended range of fuel options for MYRRHA, after the safety under both normal operation and over-power transient conditions of U-Pu MOX fuel already demonstrated in previous works from the same authors [31], [32].

The calculations performed in the present analysis focus on two irradiation scenarios, i.e., a single power cycle within the IPS position in the second ring of the MYRRHA core, and the use of Am-MOX as driver fuel along the 13 cycles of MYRRHA normal operation, along five core rings up to the final assembly discharge. Besides the reference Am content in the as-fabricated fuel (currently set at 0.49 wt.%), the possibility of increasing the Am loading to 5 wt.% (limit of the homogeneous Am recycling strategy) is accounted for and investigated within the IPS irradiation position. A significant fuel Am content implies a careful consideration of helium production and behaviour within the fuel, now coherently estimated via a surrogate model specific for the MYRRHA scenarios considered. The model is derived from synthetic datasets of helium produced under different fuel compositions and irradiation conditions corresponding to the current MYRRHA design, generated by a version of the SCIANTIX burnup module capabilities [25] extended to Am-bearing oxide fuels [26]. Moreover, updated models for fuel thermal properties, explicitly representing the effect of the Am content (besides other relevant dependencies as fuel porosity, burnup, O/M ratio, Pu content) [27] are also used to simulate the MYRRHA scenarios considered in this Deliverable, as well as advanced thermal-hydraulics boundary conditions on the MYRRHA pins from a dedicated OpenFOAM modelling of the IPS sub-channel [29] – this investigation resulting in a methodological progression towards the chaining of CFD computations with fuel pin performance evaluations. In any modelling case, the MYRRHA safety criteria (regarding the margin to fuel melting, allowed cladding plasticity and prevented outer corrosion of the cladding) are respected by wide margins.

Additional analyses herein included focus on the sensitivity of safety figures of merit to the fuel Am content compared to the impact of other relevant parameters and phenomena driving the pin performance (e.g., the gap conductance, the linear power, the coolant conditions). The latter study indicates the dominant role of the gap conductance (uncertainty and modelling) and of the thermal boundary condition provided by the coolant, while the Am effect proves to be secondary and indirect (an increasing Am loading slightly reduces the margin to fuel melting, which keeps anyway large, and contributes to the gap pressurization via the increasing helium production).

Further developments emerging from this work can be identified. From the modelling point of view, the SERPENT-informed SCIANTIX methodology for a surrogate model for helium production, herein applied to MYRRHA Am-MOX fuels, is suitable to be targeted to other fuel materials and irradiation or inter-cycle / storage conditions. The latter can be addressed via the generation and best-fit of specific artificial datasets of He production covering zero-power conditions.

Also, the present work shows the importance of focusing follow-up efforts in better assessing the gap conductance under fast reactor conditions. This is identified from the Pareto sensitivity analysis performed as a strong responsible for the fuel pin performance and hence for the associated design evaluations. Moreover, a general advancement relevant for advanced fuel performance code simulations and safety assessments under LBE (and lead) cooling environments consists in the development and use of a reliable and dedicated model for the corrosion of the cladding outer surface (specific for a certain cladding-coolant couple, besides depending on the surface temperature and on the oxygen control strategy).

The consideration of transient and accidental irradiation conditions is of high interest also from the pin performance and safety point of view, on the basis of the simulation results on Am-MOX fuels under MYRRHA normal operation herein achieved. Additionally, while the present work is limited to the "homogeneous" Am content range [0 - 5] wt.% ($(U, Pu, Am)O_{2-x}$ driver fuel design), fuel performance analyses (supported by dedicated neutronic modelling and boundary conditions) can be applied to additional fuel compositions covering the "heterogeneous" americium loading, i.e., a $(U, Am)O_{2-x}$ mixed-oxide fuel concept with Am enrichments up to 15 wt.% [39]. Since such a composition (which uses natural U) does not contain significant quantities of fissile materials, it is of interest as blanket fuel to be loaded in the outer power channels of the MYRRHA reactor core for transmutation purposes.

6 References

[1] L. F. Schlindwein and C. Montalvo, "Energy citizenship: Accounting for the heterogeneity of human behaviours within energy transition", *Energy Policy*, vol. 180, no. August 2022, 113662, 2023.

[2] M. Salvatores, "Medium and Long Term Scenarios for Fission Nuclear Energy and Role of Innovative Concepts", in: *Workshop on Nuclear Data and Nuclear Reactors: Physics, Design and Safety,* 13 March - 14 April 2000, Trieste, Italy, pp. 1–73.

[3] T. Mukaiyama, "Importance of double strata fuel cycle for minor actinide transmutation", in: *Proc. 3rd NEA Int'l Info exchange meeting on actinide and fission product partitioning and transmutation,* 12-14 December 1994, Cadarache, France, pp. 1–10.

[4] W. Weiss, C.-M. Larsson, C. McKenney, J.-P. Minon, S. Mobbs, T. Schneider, H. Umeki, W. Hilden, C. Pescatore, and M. Vesterlind, "ICRP PUBLICATION 122: Radiological Protection in Geological Disposal of Long-lived Solid Radioactive Waste", *Ann. ICRP*, vol. 42, no. 3, pp. 1–57, 2013.

[5] B. Merk, D. Litskevich, M. Bankhead, and R. J. Taylor, "An innovative way of thinking nuclear waste management - Neutron physics of a reactor directly operating on SNF", *PLoS One*, vol. 12, no. 7, e0180703, 2017.

[6] C. Poinssot, C. Rostaing, S. Grandjean, and B. Boullis, "Recycling the Actinides, The Cornerstone of Any Sustainable Nuclear Fuel Cycles", *Procedia Chem.*, vol. 7, pp. 349–357, 2012.

[7] L. Rodriguez-Penalonga and B. Y. Moratilla Soria, "A Review of the Nuclear Fuel Cycle Strategies and the Spent Nuclear Fuel Management Technologies", *Energies*, vol. 10, no. 8, p. 1235, 2017.

[8] M. Salvatores, I. Slessarev, G. Ritter, P. Fougeras, A. Tchistiakov, G. Youinou, and A. Zaetta, "Long-lived radioactive waste transmutation and the role of accelerator driven (hybrid) systems", *Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip.*, vol. 414, no. 1, pp. 5–20, 1998.

[9] A. C. Mueller, "Transmutation of Nuclear Waste and the future MYRRHA Demonstrator", *J. Phys. Conf. Ser.*, vol. 420, p. 012059, 2013.

[10] K. Fujimura, K. Kawashima, A. Sasahira, S. Itooka, H. Kiyotake, and M. Takakuwa, "High-Safety Fast Reactor Core Concepts to Improve Transmutation Efficiency of Long-lived Radioactive Waste", *Energy Procedia*, vol. 71, pp. 97–105, 2015.

[11] GIF (Generation IV International Forum), "GIF R&D Outlook for Generation IV Nuclear Energy Systems - 2018 Update", 2018.

[12] GIF (Generation IV International Forum), "Annual Report 2021", https://www.gen-4.org/gif/jcms/c_44720/annual-reports, 2021.

[13] G. Locatelli, M. Mancini, and N. Todeschini, "Generation IV nuclear reactors: Current status and future prospects", *Energy Policy*, vol. 61, pp. 1503–1520, 2013.

[14] GIF (Generation IV International Forum), "Preparing the Future through Innovative Nuclear Technology: Outlook for Generation IV Technologies", https://www.gen-4.org/gif/upload/docs/application/pdf/2019-01/preparing_the_future_through_innovative_nuclear_technology_web.pdf, 2019.

[15] European Union's Horizon 2020 Research and Innovation programme, "PATRICIA - Partitioning And Transmuter Research Initiative in a Collaborative Innovation Action", *https://patricia-h2020.eu/*, 2020.

[16] H. A. Abderrahim, D. De Bruyn, M. Dierckx, R. Fernandez, L. Popescu, M. Schyns, A. Stankovskiy, G. Van Den Eynde, and D. Vandeplassche, "MYRRHA accelerator driven system programme: Recent progress and perspectives", *Nucl. Power Eng.*, no. 2, pp. 29–41, 2019.

[17] A. Magni, A. Del Nevo, L. Luzzi, D. Rozzia, M. Adorni, A. Schubert, and P. Van Uffelen, "The TRANSURANUS fuel performance code", in: *Nuclear Power Plant Design and Analysis Codes - Development, Validation and Application*, Elsevier, Vol. III, Chap. 8, pp. 161–205, 2021.

[18] K. Lassmann, "TRANSURANUS: a fuel rod analysis code ready for use", *J. Nucl. Mater.*, vol. 188, no. C, pp. 295–302, 1992.

[19] D. Pizzocri, T. Barani, and L. Luzzi, "SCIANTIX: A new open source multi-scale code for fission gas behaviour modelling designed for nuclear fuel performance codes", *J. Nucl. Mater.*, vol. 532, 152042, 2020.

[20] G. Zullo, D. Pizzocri, and L. Luzzi, "The SCIANTIX code for fission gas behaviour: status, upgrades, separate-effect validation and future developments", *J. Nucl. Mater.*, vol. 587, 154744, 2023.

[21] P. Van Uffelen, A. Schubert, L. Luzzi, T. Barani, A. Magni, D. Pizzocri, M. Lainet, V. Marelle, B. Michel, B. Boer, S. Lemehov, and A. Del Nevo, "Incorporation and verification of models and properties in fuel performance codes", INSPYRE Deliverable D7.2, 2020.

[22] D. Pizzocri, L. Luzzi, T. Barani, A. Magni, G. Zullo, and P. Van Uffelen, "Coupling of SCIANTIX and TRANSURANUS: Simulation of integral irradiation experiments focusing on fission gas behaviour in light water reactor conditions", in: *International Workshop "Towards nuclear fuel modelling in the various reactor types across Europe"*, 28-30 June 2021, online.

[23] A. Magni, M. Di Gennaro, D. Pizzocri, G. Zullo, L. Luzzi, M. Lainet, A. Schubert, and P. Van Uffelen, "Description of new meso-scale models and their implementation in fuel performance codes", PATRICIA Deliverable D5.2, 2023.

[24] L. Luzzi, A. Magni, S. Billiet, M. Di Gennaro, G. Leinders, L. G. Mariano, D. Pizzocri, M. Zanetti, and G. Zullo, "Performance analysis and helium behaviour of Am-bearing fuel pins for irradiation in the MYRRHA reactor", *Nucl. Eng. Des.*, vol. 420, 113048, 2024.

[25] A. Cechet, S. Altieri, T. Barani, L. Cognini, S. Lorenzi, A. Magni, D. Pizzocri, and L. Luzzi, "A new burn-up module for application in fuel performance calculations targeting the helium production rate in $(U,Pu)O_2$ for fast reactors", *Nucl. Eng. Technol.*, vol. 53, pp. 1893–1908, 2021.

[26] D. Pizzocri, M. G. Katsampiris, L. Luzzi, A. Magni, and G. Zullo, "A surrogate model for the helium production rate in fast reactor MOX fuels", *Nucl. Eng. Technol.*, vol. 55, pp. 3071–3079, 2023.

[27] P. Van Uffelen, A. Schubert, M. Lainet, A. Magni, M. Di Gennaro, M. Guarnieri, D. Pizzocri, and L. Luzzi, "Description of new correlations and databases for fuel performance codes to be applied to Am bearing fuels", PATRICIA Deliverable D5.1, 2024.

[28] A. Magni, L. Luzzi, D. Pizzocri, A. Schubert, P. Van Uffelen, and A. Del Nevo, "Modelling of thermal conductivity and melting behaviour of minor actinide-MOX fuels and assessment against experimental and molecular dynamics data", *J. Nucl. Mater.*, vol. 557, 153312, 2021.

[29] A. Pérez, J. Wallenius, M. Di Gennaro, L. Luzzi, A. Magni, D. Pizzocri, X.-N. Chen, and A. Rineiski, "Towards multi-physics description of fuel behaviour for accidental conditions", PATRICIA Deliverable D5.4, 2023.

[30] P. A. Ushakov, A. V. Zhukov, and N. M. Matyukhin, "Heat transfer to liquid metals in regular arrays of fuel elements", *High Temp.*, vol. 15, no. 5, pp. 868–873, 1977.

[31] A. Magni, T. Barani, F. Belloni, B. Boer, E. Guizzardi, D. Pizzocri, A. Schubert, P. Van Uffelen, and L. Luzzi, "Extension and application of the TRANSURANUS code to the normal operating

conditions of the MYRRHA reactor", *Nucl. Eng. Des.*, vol. 386, 111581, 2022.

[32] A. Magni, M. Di Gennaro, E. Guizzardi, D. Pizzocri, G. Zullo, and L. Luzzi, "Analysis of the performance of driver MOX fuel in the MYRRHA reactor under Beam Power Jump transient irradiation conditions", *Nucl. Eng. Des.*, vol. 414, 112589, 2023.

[33] S. Lemehov, "New correlations of thermal expansion and Young's modulus based on existing literature and new data", INSPYRE Deliverable D6.3, 2020.

[34] V. Sobolev, S. Lemehov, N. Messaoudi, P. Van Uffelen, and H. Aït Abderrahim, "Modelling the behaviour of oxide fuels containing minor actinides with urania, thoria and zirconia matrices in an accelerator-driven system", *J. Nucl. Mater.*, vol. 319, pp. 131–141, 2003.

[35] M. Kato, K. Maeda, T. Ozawa, M. Kashimura, and Y. Kihara, "Physical properties and irradiation behavior analysis of Np- and Am-Bearing MOX Fuels", *J. Nucl. Sci. Technol.*, vol. 48, no. 4, pp. 646–653, 2011.

[36] D. Prieur, R. C. Belin, D. Manara, D. Staicu, J. C. Richaud, J. F. Vigier, A. C. Scheinost, J. Somers, and P. Martin, "Linear thermal expansion, thermal diffusivity and melting temperature of Am-MOX and Np-MOX", *J. Alloys Compd.*, vol. 637, pp. 326–331, 2015.

[37] L. Luzzi, T. Barani, B. Boer, L. Cognini, A. Del Nevo, M. Lainet, S. Lemehov, A. Magni, V. Marelle, B. Michel, D. Pizzocri, A. Schubert, P. Van Uffelen, and M. Bertolus, "Assessment of three European fuel performance codes against the SUPERFACT-1 fast reactor irradiation experiment", *Nucl. Eng. Technol.*, vol. 53, pp. 3367–3378, 2021.

[38] L. Luzzi, A. Magni, B. Boer, A. Del Nevo, M. Lainet, S. Lemehov, V. Marelle, B. Michel, D. Pizzocri, A. Schubert, P. Van Uffelen, and M. Bertolus, "Assessment of INSPYRE-extended fuel performance codes against the SUPERFACT-1 fast reactor irradiation experiment," *Nucl. Eng. Technol.*, vol. 55, no. 3, pp. 884–894, 2023.

[39] E. D'Agata, P. R. Hania, D. Freis, J. Somers, S. Bejaoui, F. F. Charpin, P. J. Baas, R. A. F. Okel, S. van Til, J. M. Lapetite, and F. Delage, "The MARINE experiment: Irradiation of sphere-pac fuel and pellets of UO_{2-x} for americium breading blanket concept", *Nucl. Eng. Des.*, vol. 311. pp. 131–141, 2017.

[40] OECD/NEA, *Handbook on Lead-bismuth Eutectic Alloy and Lead Properties, Materials Compatibility, Thermal- hydraulics and Technologies*, 2015 Edition, Technical Report NEA No. 7268, 2015.

[41] K. Mikityuk, "Heat transfer to liquid metal: Review of data and correlations for tube bundles", *Nucl. Eng. Des.*, vol. 239, no. 4, pp. 680–687, 2009.

[42] M. Di Gennaro, A. Magni, M. Mastrogiovanni, D. Pizzocri, and L. Luzzi, "OpenFOAM-informed TRANSURANUS simulation of the fuel pin behaviour in the MYRRHA reactor during BPJ transient scenario", in: *16th Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation (16IEMPT)*, 24-27 October 2023, NEA Headquarters, Boulogne-Billancourt, France.

[43] D. Pizzocri, A. Magni, G. Zullo, and L. Luzzi, "SCIANTIX open-source code for fission gas behaviour: objectives and foreseen developments", in: *IAEA Technical Meeting on the Development and Application of Open-Source Modelling and Simulation Tools for Nuclear Reactors (ONCORE)*, 22-24 June 2022, Milano, Italy.

[44] D. Pizzocri, T. Barani, L. Luzzi, A. Magni, G. Zullo, "The SCIANTIX grain-scale code: recent developments for high burnup fuels", in: *IAEA Technical Meeting on Safety and Performance Aspects in the Development and Qualification of High Burnup Nuclear Fuels for Water-Cooled Reactors*, 15-18 November 2022, IAEA Headquarters, Vienna, Austria.

[45] D. Pizzocri, T. Barani, and L. Luzzi, “Coupling of TRANSURANUS with the SCIANTIX fission gas behaviour module”, in: *International Workshop “Towards Nuclear Fuel Modelling in the Various Reactor Types Across Europe”*, 18-19 June 2019, Karlsruhe, Germany.

[46] G. Zullo, D. Pizzocri, A. Magni, P. Van Uffelen, A. Schubert, and L. Luzzi, “Towards grain-scale modelling of the release of radioactive fission gas from oxide fuel. Part II: Coupling SCIANTIX with TRANSURANUS”, *Nucl. Eng. Technol.*, vol. 54, no. 12, pp. 4460–4473, 2022.

[47] G. Zullo, D. Pizzocri, L. Luzzi, F. Kremer, R. Dubourg, A. Schubert, and P. Van Uffelen, “Towards simulations of fuel rod behaviour during severe accidents by coupling TRANSURANUS with SCIANTIX and MFPR-F,” *Ann. Nucl. Energy*, vol. 190, no. March, 109891, 2023.

[48] A. Magni, D. Pizzocri, L. Luzzi, M. Lainet, and B. Michel, “Application of the SCIANTIX fission gas behaviour module to the integral pin performance in sodium fast reactor irradiation conditions”, *Nucl. Eng. Technol.*, vol. 54, pp. 2395–2407, 2022.

[49] A. Magni, T. Barani, A. Del Nevo, D. Pizzocri, D. Staicu, P. Van Uffelen, and L. Luzzi, “Modelling and assessment of thermal conductivity and melting behaviour of MOX fuel for fast reactor applications”, *J. Nucl. Mater.*, vol. 541, 152410, 2020.

[50] M. L. Grossbeck, K. Ehrlich, and C. Wassilew, “An assessment of tensile, irradiation creep, creep rupture, and fatigue behavior in austenitic stainless steels with emphasis on spectral effects”, *J. Nucl. Mater.*, vol. 174, no. 2–3, pp. 264–281, 1990.

[51] S. E. Lemehov, V. P. Sobolev, and M. Verwerft, “Predicting thermo-mechanical behaviour of high minor actinide content composite oxide fuel in a dedicated transmutation facility”, *J. Nucl. Mater.*, vol. 416, no. 1–2, pp. 179–191, 2011.

[52] A. Magni, M. Bertolus, M. Lainet, V. Marelle, B. Michel, A. Schubert, P. Van Uffelen, L. Luzzi, D. Pizzocri, B. Boer, S. Lemehov, and A. Del Nevo, “Fuel performance simulations of ESNII prototypes: Results on the MYRRHA case study”, INSPYRE Deliverable D7.5, 2022.

[53] P. Botazzoli, L. Luzzi, S. Brémier, A. Schubert, P. Van Uffelen, C. T. Walker, W. Haeck, and W. Goll, “Extension and validation of the TRANSURANUS burn-up model for helium production in high burn-up LWR fuels”, *J. Nucl. Mater.*, vol. 419, no. 1–3, pp. 329–338, 2011.

[54] European Commission, *TRANSURANUS Handbook*, Joint Research Centre, Karlsruhe, Germany, 2022.

[55] G. Pastore, L. Luzzi, V. Di Marcello, and P. Van Uffelen, “Physics-based modelling of fission gas swelling and release in UO_2 applied to integral fuel rod analysis”, *Nucl. Eng. Des.*, vol. 256, pp. 75–86, 2013.

[56] L. Wilkinson, “Revising the Pareto Chart”, *Am. Stat.*, vol. 60, no. 4, pp. 332–334, 2006.

[57] X. Franch, R. S. Kenett, A. Susi, N. Galanis, R. Glott, and F. Mancinelli, “Chapter 14 - Community Data for OSS Adoption Risk Management”, in: *The Art and Science of Analyzing Software Data*, Elsevier, Chap. 14, pp. 377–409, 2016.

[58] M. Alkiayat, “A Practical Guide to Creating a Pareto Chart as a Quality Improvement Tool”, *Glob. J. Qual. Saf. Healthc.*, vol. 4, no. 2, pp. 83–84, 2021.

[59] K. Lassmann and F. Hohlefeld, “The revised URGAP model to describe the gap conductance between fuel and cladding”, *Nucl. Eng. Des.*, vol. 103, no. 2, pp. 215–221, 1987.

[60] M. Charles and M. Bruet, “Gap conductance in a fuel rod: Modelling of the FURET and CONTACT results”, in: *IAEA Specialists' Meeting on water reactor fuel element performance computer modeling*, 9-13 April 1984, Bowness-on-Windermere, United Kingdom.

[61] G. Pastore, “Modelling of Fission Gas Swelling and Release in Oxide Nuclear Fuel and Application to the TRANSURANUS Code”, PhD Thesis, Politecnico di Milano, Italy, 2012.

[62] L. Luzzi, A. Cammi, V. Di Marcello, S. Lorenzi, D. Pizzocri, and P. Van Uffelen, “Application of the TRANSURANUS code for the fuel pin design process of the ALFRED reactor”, *Nucl. Eng. Des.*, vol. 277, pp. 173–187, 2014.

[63] W. Dienst, I. Muelle-Lyda, and H. Zimmermann, “Swelling, densification and creep of oxide and carbide fuels under irradiation”, in: *International conference on fast breeder reactor performance,* 5-8 March 1979, Monterey, California, USA, pp. 166–175.

[64] C. F. Clement, “The movement of lenticular pores in UO_2 nuclear fuel elements”, *J. Nucl. Mater.*, vol. 68, no. 1, pp. 63–68, 1977.