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A methodology for accelerated design of irradiation experiments: Demonstration via an OpenFOAM-informed TRANSURANUS simulation

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A B S T R A C T

The design and licensing of irradiation experiments typically require dedicated neutronics, thermo-hydraulics, and thermo-mechanical simulations, among which neutronics and thermo-hydraulics present considerable computational burdens. In this work, we propose a methodology to potentially reduce the required number of simulations, thus accelerating the design of irradiation experiments. The proposed methodology is based on the systematic comparison of intrinsic modelling uncertainties of relevant figures of merit with either the impact of the reciprocal influence of neutronics, thermo-hydraulics, and thermo-mechanics, or the impact of design parameters of the irradiation experiment itself. We exemplify the application of the proposed methodology on the design of irradiation experiments with varying americium content in the in-pile test section of the MYRRHA research fast reactor, demonstrating the possibility of reducing the number of required thermo-hydraulic and thermo-mechanic simulations.

1. Introduction

For a better utilization of natural resources and improvements of the nuclear waste management process, current strategies foresee the introduction of fast reactors as a part of the nuclear reactor fleet, paired with the use of innovative nuclear fuels, like minor actinide-bearing mixed oxides, and structural materials able to face extreme operative conditions (high temperature, increase in-core residence time, exposure to fast neutron flux, challenging radiation loads on in-core materials and chemically aggressive coolant environment) ([Stanculescu,](#page-6-0) [2018;](#page-6-0) [Pioro](#page-6-1), [2023](#page-6-1); [Waltar et al.,](#page-6-2) [2012](#page-6-2)).

The development and qualification of new materials capable of withstanding these operative conditions in the reactor core is generally achieved by performing irradiation experiments in appropriate facilities ([Cetiner et al.](#page-6-3), [2016](#page-6-3)), demonstrators [\(Gabrielli et al.,](#page-6-4) [2015](#page-6-4)) or in-pile test section sub-assemblies ([IAEA,](#page-6-5) [2014\)](#page-6-5) as representative as possible of the in-reactor conditions and able to reproduce variable operational conditions ([Beausoleil et al.](#page-6-6), [2021](#page-6-6)).

The approval process for conducting an irradiation experiment encompasses both its design and qualification aspects supported by modelling and simulation activities, which aim to assess the performance and behaviour of the materials or systems under irradiation conditions [\(Terrani et al.,](#page-6-7) [2020\)](#page-6-7). These simulation-based methodologies play a crucial role in the regulatory approval process by providing insights into the expected outcomes, safety margins, and overall effectiveness of the experiment, ultimately contributing to the successful implementation of irradiation campaigns ([Aguiar et al.](#page-6-8), [2020](#page-6-8)).

To provide a comprehensive understanding of the complex interactions among various physical aspects inherent to an irradiation experiment (neutronics, thermo-hydraulics, fuel behaviour and structural mechanics), a multi-physics approach with an adequate level of resolution is essential [\(Demazière,](#page-6-9) [2020\)](#page-6-9). This modelling approach requires the combination of computational fluid dynamics (CFD) codes for thermo-hydraulics, Monte Carlo or deterministic codes for neutronics and fuel performance codes for pin behaviour. The bottleneck in this approach lies in the higher modelling and computational costs associated with high-fidelity thermo-hydraulic and neutronics simulations when compared to the computational requirements of fuel performance codes ([Wang et al.,](#page-6-10) [2020](#page-6-10); [Van Uffelen et al.](#page-6-11), [2019\)](#page-6-11).

In this work, we propose and demonstrate a methodology that aims to minimize the number of high-fidelity simulations required to design an irradiation experiment. The reduction of the computational burden is ensured by performing the thermo-hydraulic simulations once (offline, before the fuel performance analysis) and utilizing the obtained results online (provided as input) during the thermo-mechanical analysis performed with fuel performance codes. The validity of this approach lies in demonstrating that the impact of the thermo-mechanical analysis on the fluid dynamics is considerably smaller than the intrinsic uncertainties on the pin thermo-mechanics.

The proposed methodology is demonstrated on an irradiation experiment designed to be hosted in the in-pile test section (IPS) subassembly of the MYRRHA reactor (core design revision 1.8 ([Luzzi](#page-6-12)

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[et al.,](#page-6-12) [2024;](#page-6-12) [Perez et al.,](#page-6-13) [2023](#page-6-13))) selected as a case study. The purpose of this experiment is to test mixed-oxide fuel with different contents of americium (up to 5 wt.%) to be irradiated in the MYRRHA reactor. The IPS irradiation scenarios under consideration include both normal operation and transient (beam power jump, BPJ) conditions. The thermomechanical simulations are performed with the TRANSURANUS fuel performance code ([Lassmann](#page-6-14), [1992](#page-6-14); [Magni et al.,](#page-6-15) [2021b](#page-6-15)) informed by thermo-hydraulic boundary conditions evaluated via the computational fluid dynamics software OpenFOAM [\(OpenFOAM,](#page-6-16) [2018](#page-6-16)).

The paper is organized as follows. Section [2](#page-1-0) is dedicated to outlining the herein proposed methodology. In Section [3,](#page-2-0) the simulation setup is outlined, providing a description of the selected case study and the codes employed for conducting thermo-hydraulic and thermomechanical simulations. Then, in Section [4](#page-3-0) the proposed methodology is demonstrated. Conclusions and future perspectives arising from this work are provided in Section [5.](#page-4-0)

2. Description of the proposed methodology

The authorization to conduct an irradiation experiment, aimed at the qualification of nuclear fuel pin designs, deals with the safety and design of the experimental setup itself [\(Crawford et al.](#page-6-17), [2007](#page-6-17)). The commonly adopted methodology [\(Fig.](#page-2-1) [1\(a\)](#page-2-1)) formally requires performing an iterative procedure between irradiation experiment design and scenario calculations. Initially, the irradiation experiment design is set up, encompassing considerations such as materials, desired temperature, irradiation duration, fuel composition, target dose and neutron spectrum (connected to the experiment position within the reactor core). This procedure aims to meet a set of objectives pertaining to the experiment's functionality, performance, and safety ([Tirel et al.](#page-6-18), [2022\)](#page-6-18). Then, the experimental design parameters (e.g., the plutonium or americium content in the fuel, the cladding material or the operative conditions) are defined (denoted as x_i and formally indexed from $i = 0$ to P in the internal loop outlined in [Fig.](#page-2-1) [1\(a\)\)](#page-2-1). Subsequently, the defined irradiation experiment undergoes evaluation through numerical simulations, to predict the performance of materials in the specific environment, aiding in the set-up to ensure both the safety of the experiment and the acquisition of meaningful data [\(Terrani et al.,](#page-6-7) [2020](#page-6-7)). For each experimental design parameter, appropriate and critical figures of merit (FOM) are identified from among the quantities of interest for safety, to assess compliance with safety limits (like the margin to fuel melting and the outer cladding temperature against corrosion). To investigate the inter-dependency between different physics involved in an irradiation experiment (neutronics, thermo-hydraulics, fuel behaviour and structural mechanics^{[1](#page-1-1)}) for a more in-depth understanding of the system behaviour, it is formally necessary to adopt a high-resolution multi-physics approach ([Demazière,](#page-6-9) [2020\)](#page-6-9). Typically, high-fidelity simulations are sequenced since the expected feedback is low. When possible, neutronics (N) simulations are performed first and used to inform thermo-hydraulics (T/H) simulations. In turn, information coming from both neutronics (power and flux) and thermo-hydraulics (temperature boundary conditions) are used to perform thermo-mechanics (T/M) (see [Fig.](#page-2-1) $1(a)$). Performing high-fidelity neutronic and thermohydraulic simulations is demanding from both the computational time and cost points of view, posing challenges when multiple assessments or real-time analyses are essential ([Wang et al.,](#page-6-10) [2020\)](#page-6-10). Instead, the thermo-mechanical analysis typically relying on 1.5D or 2D fuel performance codes requires a lower computational burden ([Van Uffelen](#page-6-11) [et al.,](#page-6-11) [2019](#page-6-11)).

In this work, we thus propose a methodology (outlined in [Fig.](#page-2-2) $1(b)$) to reduce the number of high-fidelity neutronics and thermo-hydraulics

simulations required to design an irradiation experiment.^{[2](#page-1-2)} Instead of repeating high-fidelity neutronics and thermo-hydraulics calculations for each value of experimental design parameters, we propose to first analyse extreme values (again, formally $i = 0$ and $i = P$ in [Fig.](#page-2-2) [1\(b\)\)](#page-2-2) and to compare them with intrinsic uncertainties on the relevant figures of merit to determine the need to perform further high-fidelity analyses. We propose the notation $\{T/M_i|T/H_j;N_j\}$ to account with which *i* and j values of an experimental design parameter the thermo-hydraulics, neutronics, and thermo-mechanics calculations are performed.[3](#page-1-3) With this notation $FOM_{0|0}$ represents a figure of merit calculated with thermo-hydraulics, neutronics, and thermo-mechanics all referring to the value $i = 0$ of the experimental design parameter. The founding idea of the proposed methodology is to compare the variation of a figure of merit due to the impact of different values of experimental design parameters on the simulations with the intrinsic uncertainty on the figure of merit itself. Formally the first comparison is with the extreme values of the experimental design parameters ([Fig.](#page-2-2) [1\(b\)\)](#page-2-2), i.e.

$$
FOM_{P|P} - FOM_{P|0} < \sigma_{FOM} \tag{1}
$$

in which the figure of merit is calculated with thermo-mechanics simulation coherent with the experimental design parameter $P\left\{\cdot, \right.$ given high-fidelity simulations performed with either coherent \cdot | P or reference ⋅|0 values of the experimental design parameter. If the impact on the figure of merit of not informing the thermo-mechanics simulation with coherent (in terms of value of experimental parameters) highfidelity simulations is less than the intrinsic uncertainty on the figure of merit itself, one can assume that the reference high-fidelity simulations ⋅|0 can be kept valid and thus only the thermo-mechanics calculations are to be repeated for each value of the experimental design parameter $i|0.$

With intrinsic uncertainty we refer to the variability of the selected figure of merit considering the uncertainty of input parameters. These input parameters, whose uncertainties significantly impact the figure of merit, can be identified through sensitivity analysis.^{[4](#page-1-4)} The intrinsic uncertainty of the chosen FOM, σ_{FOM} , is quantified by propagating the uncertainty of all parameters.

The chosen case study for illustrating the proposed methodology involves designing experiments within the in-pile test section subassembly of the MYRRHA reactor with varying americium content (up to 5 wt.%, Section [3.1](#page-2-3)). The analysis encompasses both the normal operation and a postulated transient scenario relevant to the MYRRHA reactor, i.e., the beam power jump.^{[5](#page-1-5)}

 $^{\rm 1}$ Other physics such as coolant chemistry and radio-nuclide transport are not considered here, but depending on the considered experiment can be added to the picture.

² As mentioned, a prior step for the application of the proposed methodology is to demonstrate that neutronics, thermo-hydraulics, and thermomechanics can be decoupled. This is typically true, despite very specific designs and scenarios (e.g., [Holt et al.,](#page-6-19) [2015\)](#page-6-19), but nevertheless we will consider this step in the following case study. To decouple the neutronics and thermohydraulics calculations from the thermo-mechanical one, we look at the impact of the thermo-mechanical analysis on fluid dynamics and neutronics. Such impact is compared with the intrinsic uncertainties of identified figures of merit.

³ Formally this notation considers the thermo-mechanical calculation to be performed given a set of high-fidelity simulation, either with or without coherent experimental design parameters.

⁴ It is worth recalling that the knowledge of the impact of each parameter on critical figures of merit is a requirement of the qualification of nuclear software ([Autorité de Sûreté Nucléaire,](#page-6-20) [2017\)](#page-6-20), and thus these tools are typically equipped with methods for sensitivity analysis and uncertainty propagation.

⁵ Without lack of generality, in this case study we do not consider the impact of neutronics on both thermo-hydraulics and thermo-mechanics. As a reference, the impact on the local power and fluxes of variations in the concentration of americium, up to 5 wt.%, in the in-pile test section sub-assembly is calculated and shown in [Pizzocri et al.](#page-6-21) [\(2024\)](#page-6-21).

(a) Flowchart of the current methodology

(b) Flowchart of the proposed methodology

Fig. 1. Illustration of the flowchart of the simulations (N stands for neutronics, T/H for thermo-hydraulics, and T/M for thermo-mechanics) required for the design of irradiation experiments in the (a) current methodology and the (b) proposed methodology. In the proposed methodology, the support of an uncertainty analysis can reduce the number of high-fidelity simulations to be performed, within a range of experimental design parameters.

3. Simulation of the case study

In this section, as a case study for an irradiation experiment location, the in-pile test section (IPS) sub-assembly of the MYRRHA reactor is delineated, encompassing details of the irradiation history and specifications of the analysed over-power transient scenario, and the codes employed for conducting thermo-hydraulic and thermomechanical simulations are presented. In the following section we will details examples of experimental activities to be performed in the IPS and apply the proposed methodology to them.

3.1. Case study

The IPS sub-assemblies are hosted in the sub-critical (accelerationdriven) configuration (70 MWth thermal power) of the MYRRHA reactor (core design version 1.8, [Fig.](#page-3-1) [2](#page-3-1)) and dedicated to experimental irradiation under fast neutron fluxes of innovative americium-bearing fuel pins (as driver or blanket pins) ([Fiorito et al.,](#page-6-22) [2021\)](#page-6-22). These experimental sub-assemblies are located in the second concentric ring of the core, around the lead-bismuth eutectic (LBE) spallation target.^{[6](#page-2-4)} According to the designed MYRRHA operative schedule, the IPS ''unit'' irradiation consists of 90 days of single-cycle at full reactor power.

Besides normal operation conditions, to design and license an irradiation experiment one needs to consider also off-normal conditions. As a representative example for the MYRRHA IPS, we consider the occurrence of a beam power jump (BPJ), i.e., a fast over-power transient scenario triggered by an over-current of the external proton accelerator coupled with the MYRRHA sub-critical core.^{[7](#page-2-5)} Various BPJs scenarios can be considered, as they have the potential to occur at any moment during normal reactor operation—at the beginning, during or at the end of the single-cycle IPS normal irradiation. In this work, the representative BPJ transient selected to demonstrate the validity and applicability of the methodology proposed (Section [2\)](#page-1-0), is assumed to take place at the end of the IPS normal operation. The maximum (at the axial peak power node and for the hottest pin) linear heat rate and fast neutron flux history during the MYRRHA-IPS normal irradiation and BPJ transient are reported in [Fig.](#page-3-2) [3,](#page-3-2) based on data provided by SCK CEN, in the framework of the PATRICIA Project [\(European Union's](#page-6-23) [Horizon,](#page-6-23) [2020\)](#page-6-23), holding for the reference Am-MOX composition (0.49 wt.% americium and 29.51 wt.% plutonium). 8

⁶ The reader is referred to [Luzzi et al.](#page-6-12) ([2024\)](#page-6-12) and to [Perez et al.](#page-6-13) [\(2023\)](#page-6-13) for complete details about the MYRRHA fuel pin specifications.

⁷ For a comprehensive understanding of the details regarding the beam power jump transient scenario, the reader is referred to [Magni et al.](#page-6-24) ([2023\)](#page-6-24) and [Di Gennaro et al.](#page-6-25) [\(2023](#page-6-25)).

⁸ Typically, it is anticipated that during the BPJ transient, if the high neutron flux signal persists for over 3 s, it prompts the accelerator and reactor to shut down within a 3-second window. In this work, we explore a hypothetical scenario where the BPJ transient extends beyond 3 s, at which the reactor scram should occur.

Fig. 2. MYRRHA sub-critical core layout according to the current design ''Revision 1.8''.

Fig. 3. Linear heat rate and fast neutron flux (energy *>* 0.1 MeV) at the axial peak power node of the hottest pin, corresponding to the specifications of MYRRHA ''Revision 1.8'' under IPS normal operation and BPJ transient scenarios.

3.2. Thermo-hydraulic modelling of the IPS sub-channel

In the proposed application, the high-fidelity computational fluid dynamics simulation of the MYRRHA-IPS sub-channel is performed using the open-source code OpenFOAM version 6 [\(OpenFOAM,](#page-6-16) [2018](#page-6-16)), which solves the governing equations using the Finite-Volume method ([Moukalled et al.](#page-6-26), [2016](#page-6-26)). The analysis is carried out on the interior sub-channel of the IPS sub-assembly without considering the presence of the wire-wrapper. The dynamics of the LBE flow are solved using the standard incompressible Navier–Stokes equations coupled with the energy equation under the Boussinesq approximation for density. The solver adopted corresponds to the bouyantBoussinesqPimple-Foam available in the OpenFOAM version adopted here, appropriately modified to accurately capture the LBE-coolant flow conditions in the MYRRHA-IPS sub-channel ([OECD/NEA](#page-6-27), [2015\)](#page-6-27). The fuel power is prescribed as a fixed input based on the data provided by SCK CEN ([Fig.](#page-3-1) [2](#page-3-1)), and it follows the dynamics governed by the specific heat of the fuel obtained from the TRANSURANUS simulation described in Section [3.3.](#page-3-3) Turbulence is modelled using the linear eddy viscosity

model $k - \omega$ SST [\(Menter](#page-6-28), [1994\)](#page-6-28), employed in the low Reynolds formulation. The heat transfer is modelled adopting the gradient diffusion assumption ([Shams and De Santis](#page-6-29), [2019](#page-6-29)), and considers the local model proposed by Kays in [Kays](#page-6-30) ([1994\)](#page-6-30) for the turbulent Prandtl number. For the sake of brevity, the specification of the mesh and numerical settings are not provided here, as it has already been thoroughly discussed in [Di](#page-6-31) [Gennaro](#page-6-31) [\(2023](#page-6-31)), [Di Gennaro et al.](#page-6-25) ([2023\)](#page-6-25), and in [Perez et al.](#page-6-13) ([2023](#page-6-13)).

The thermo-hydraulics boundary conditions of interest transferred to the thermo-mechanics fuel performance code, i.e., TRANSURANUS (see next sub-section), are the cladding outer temperature and the pressure drops. Precision in assessing the cladding outer temperature is essential for a deeper comprehension of cladding swelling, creep, and corrosion, which are temperature and irradiation driven.

3.3. Thermo-mechanical modelling of the IPS fuel pin

In our application, the thermo-mechanical simulations of the MYRRHA-IPS fuel pin are performed with the TRANSURANUS fuel performance code. The code version adopted in this work, v1m4j22, is equipped with suitable models for the properties of MYRRHA pin materials (fuel and cladding, while the coolant is treated by Open-FOAM). For modelling the mechanical properties (thermal expansion and Young's modulus) of Am-MOX fuels the correlations proposed in [Lemehov](#page-6-32) [\(2020](#page-6-32)) are used, while for the thermal properties (thermal conductivity and melting temperature) the ones proposed by [Magni](#page-6-33) [et al.](#page-6-33) ([2021a\)](#page-6-33) are adopted covering the ranges associated to the MYRRHA irradiation in terms of temperature, Am and Pu contents, deviation from stoichiometry, porosity, and burnup. The fuel specific heat is modelled by adopting the correlation reported in [Chawla et al.](#page-6-34) ([1981\)](#page-6-34). The behaviour of inert gases (xenon, krypton, and helium) within the fuel matrix is modelled in TRANSURANUS via the grain scale code SCIANTIX [\(Pizzocri et al.,](#page-6-35) [2020;](#page-6-35) [Zullo et al.,](#page-6-36) [2023\)](#page-6-36). This multi-scale framework enables a comprehensive calculation of fuel swelling and gas release in the fuel-cladding gap resulting from the intra- and inter-granular description of the gas dynamics employing mechanistic approaches based on kinetic rate-theory models. Moreover, SCIANTIX has also been recently equipped with a surrogate model for helium production dedicated to the MYRRHA IPS fuel composition and irradiation conditions ([Luzzi et al.,](#page-6-12) [2024](#page-6-12)). For the MYRRHA cladding austenitic steel phenomena, TRANSURANUS is equipped with recently developed correlations for the thermal and irradiation-induced creep strain, void swelling, and thermal creep time-to-rupture, applicable to ranges relevant for the current MYRRHA core design [\(Magni et al.](#page-6-37), [2022\)](#page-6-37).

4. Demonstration of the proposed methodology

In this section, the methodology proposed in Section [2](#page-1-0) is demonstrated. In this work, the experimental design parameter i of [Fig.](#page-2-2) [1\(b\)](#page-2-2) corresponds to the americium content in the MOX fuel. The variation considered here falls within the range of the homogeneous fuel strategy, from 0.49 wt.% Am (with 29.51 wt.% Pu), which represents the reference for the current MYRRHA design (namely the 0 of [Fig.](#page-2-2) [1\(b\)](#page-2-2)), to 5 wt.% Am (with 25 wt.% Pu) (namely the P of [Fig.](#page-2-2) [1\(b\)](#page-2-2)). In Section [4.1](#page-4-1), the first part of the scheme shown in [Fig.](#page-2-2) [1\(b\)](#page-2-2) is outlined, focusing on the possibility of reducing the number of high-fidelity thermohydraulics calculations needed for each value of the americium content, by demonstrating the possibility of decoupling thermo-hydraulics and thermo-mechanics. Then, in Section [4.2](#page-4-2), the second aspect of the methodology is illustrated, which explores the possibility of reducing the number of thermo-mechanical simulations needed for each value of the americium content.

4.1. Decoupling of thermo-hydraulics and thermo-mechanics

Given the LBE cooling environment, the figure of merit selected to show the possibility of neglecting the inter-dependency between thermo-mechanical analysis and thermo-hydraulic one is the cladding outer temperature on which a design limit is set to prevent external cladding corrosion from the coolant [\(Luzzi et al.](#page-6-12), [2024\)](#page-6-12).

In this case, where the impact of neutronics on both thermohydraulics and thermo-mechanics is not considered, the americium content does not affect the cladding outer temperature. The only thing that affects the thermo-hydraulic calculation is the geometrical deformation of the fuel pin affecting the coolant channel and consequently the pin coolability. During the IPS normal and transient simulation, as the temperature progressively increases along the fuel pin height, the outer radius of the cladding undergoes radial expansion. The maximum variation predicted by TRANSURANUS is 0.025 mm (going from 3.275 mm to 3.3 mm for the cladding outer radius), in correspondence of the maximum active height of the fuel column. This deformation induces a reduction of the hydraulic diameter of the coolant channel, which in turn affects the velocity of the coolant, the heat transfer coefficient and the pressure drops.

In order to quantitatively evaluate the impact of the fuel pin expansion on the cladding temperature, the shrinked IPS sub-channel was simulated in OpenFOAM considering the maximum radius predicted by TRANSURANUS (namely 3.3 mm). It was possible to notice that the expansion on the cladding outer radius leads to an increase of the LBE velocity, going from 1.84 to 1.88, a slight reduction of the cladding outer temperature, depicted by the orange dotted line in [Fig.](#page-5-0) [4,](#page-5-0) and slightly higher pressure drops (from 0.114 MPa to 0.119 MPa).

The intrinsic uncertainty on the cladding outer temperature is derived by propagating the uncertainty on the LBE Nusselt number, whose value is reported in [Table](#page-5-1) [1.](#page-5-1) As illustrated in [Fig.](#page-5-0) [4,](#page-5-0) within the uncertainty range associated with this figure of merit, both the calculation with the original geometry and the shrinked one are indistinguishable. It can be concluded that the structural feedback on fluid dynamics does not significantly impact the thermo-hydraulics simulations performed in OpenFOAM. For this reason, as indicated by the proposed methodology (Section [2\)](#page-1-0) through Eq. [\(1\)](#page-1-6), it is feasible to decouple these two phases and to perform a single fluid dynamics calculation valid for different pin performance scenarios (associated with the MYRRHA irradiation case considered in this work).

4.2. Minimization of thermo-mechanical simulations

From the thermo-mechanical analysis conducted on the MYRRHA-IPS fuel pin in [Luzzi et al.](#page-6-12) ([2024\)](#page-6-12), the Von Mises equivalent stress in the cladding is well below the cladding yield stress. This is attributed to the absence of fuel-cladding mechanical interaction (gap closure) and the relatively minor impact of pressure loadings on the cladding (the maximum pressure in the gap turns out to be 0.19 MPa, whereas the maximum coolant pressure occurs at the inlet of the sub-channel and corresponds to 0.6 MPa), along with the fact that the thermal gradient across the cladding is not significant (approximately a maximum temperature change of 20 ◦C). For these reasons, the design limit on the plastic strain of the cladding, allowed up to 0.5% ([Magni et al.](#page-6-37), [2022\)](#page-6-37), is fully respected. Consequently, the only figure of merit under consideration in the analysis is the fuel central temperature (highly influenced by the americium content), whose value must be kept under control in order to keep a sufficient margin to fuel melting (design limit of 2600 ◦C imposed on the maximum fuel temperature) ([Magni et al.](#page-6-37), [2022\)](#page-6-37).

The two main parameters that can impact the safety-related fuel central temperature are the gap conductance and thermal conductivity of the fuel, as evidenced by the sensitivity analysis conducted in [Luzzi](#page-6-12) [et al.](#page-6-12) ([2024\)](#page-6-12). By propagating the uncertainty associated with these two parameters, reported in [Table](#page-5-1) [1](#page-5-1), the intrinsic uncertainty on fuel

central temperature is evaluated [\(Table](#page-5-1) [1\)](#page-5-1). Following the proposed methodology outlined in Section [2,](#page-1-0) the first comparison is conducted using the extreme values of the homogeneous strategy range, specifically 0.49 wt.% and 5 wt.% of americium, as shown in [Fig.](#page-5-2) [5](#page-5-2). It is possible to notice the strong temperature variation in the fuel induced by the americium content, as already attested in [Luzzi et al.](#page-6-12) ([2024\)](#page-6-12) and caused by the degradation of fuel thermal conductivity by americium ([Magni et al.](#page-6-33), [2021a\)](#page-6-33). Despite this, even in the worst case with 5 wt.% of americium, the fuel central temperature is largely within the uncertainty range. It is possible to conclude that the suitability and safety of the fuel pin design are confirmed leading to the possibility of extending the experiment licensing to experiments involving an americium content included within the range corresponding to the homogeneous recycling strategy (0.49 wt.% - 5 wt.%), without the need to repeat the thermo-mechanical analysis.

A single OpenFOAM simulation of the IPS sub-channel during normal operation and BPJ transient takes approximately one day on an Intel Core i9-10980XE CPU @ 3.00 GHz, whereas the TRANSURANUS simulation lasts about 3 min. Coupling these two phases would necessitate performing CFD calculations each time there is a deformation of the external radius of the cladding, leading to a total computational effort spanning several days. Moreover, this computational burden escalates when simulating the behaviour of different americium contents in the fuel. Having demonstrated the ability to decouple the thermomechanical and thermo-hydraulic calculations (Section [4.1\)](#page-4-1), as well as the possibility of minimizing the number of thermo-mechanical simulations needed for each value of the americium content (Section [4.2](#page-4-2)), significantly reduces the computational cost to just one day for this specific case study.

5. Conclusions

In this work, we presented a methodology to accelerate the design of irradiation experiment and thus the qualification process. The methodology aims at minimizing the overall number of neutronics, thermohydraulics and thermo-mechanical simulations typically required to license irradiation experiments, relying on a systematic comparison between the impact of the reciprocal influence of these physics or the impact of design parameters of the experiment on selected figures of merit, and the intrinsic modelling uncertainties associated with such figures of merit.

The effectiveness of this methodology is showcased through its application on the design of irradiation experiments with varying americium content (up to 5 wt.%) in the in-pile test section sub-assembly of the MYRRHA research fast reactor, encompassing both normal irradiation conditions and a postulated over-power transient scenario, i.e., the beam power jump. Thermo-mechanical simulations were performed with the TRANSURANUS fuel performance code, informed by thermohydraulic boundary conditions (i.e., pressure drops and cladding outer temperature) evaluated via the computational fluid dynamics software OpenFOAM.

For the specific case under investigation, the relevant figures of merit selected are the cladding outer temperature and the fuel central temperature, for which design limits are set to prevent external cladding corrosion and fuel melting. From the uncertainty analysis conducted on these two figures of merit is possible to conclude that: (i) the influence of structural feedback on fluid dynamics has a negligible impact on thermo-hydraulic simulations, making it feasible to decouple these two phases; (ii) the suitability and safety of the inpile test section experiment design for different americium contents is confirmed, without the necessity to repeat the thermo-mechanical analysis, as long as the americium content remains within the range corresponding to the homogeneous recycling strategy (0.49 wt.%–5 wt.%). Overall, this results in a saving of several days of computational effort for the specific case study being considered.

Fig. 4. Comparison between the cladding outer temperature predicted via OpenFOAM with the original sub-channel geometry and the shrinked one resulting from the fuel pin expansion predicted by TRANSURANUS. The comparison is shown both during normal operation (on the left) and the over-power transient scenario (on the right), depicting steady-state conditions. In blue is reported the uncertainty band on the cladding outer temperature evaluated propagating the uncertainty on the LBE Nusselt number reported in [Table](#page-5-1) [1](#page-5-1).

Fig. 5. Comparison between the fuel central temperature evaluated for two different fuel Am contents (0.49 wt.%–5 wt.%). The comparison is shown both during normal operation (on the left) and the over-power transient scenario (on the right). In blue is reported the uncertainty band on the fuel central temperature evaluated propagating the uncertainty on the gap conductance and fuel thermal conductivity reported in [Table](#page-5-1) [1.](#page-5-1)

Table 1

List of parameters and their uncertainties, taken from [Luzzi et al.](#page-6-12) ([2024\)](#page-6-12), along with the intrinsic uncertainty on the selected FOM obtained by propagating the uncertainties associated with these parameters.

In conclusion, the methodology developed in this paper, when applicable, proves effective in accelerating the computational analyses required to support the design and approval process for experimental campaigns, and exhibits the potential for wider application to various in-reactor irradiation experiments. This methodology can also be effectively extended to fuel and core design as well. This flexibility can make it a valuable tool for designers to optimize fuel performance and core safety, addressing complex interactions and reducing the computational effort needed for comprehensive analysis.

CRediT authorship contribution statement

M. Di Gennaro: Writing – original draft, Software, Methodology, Conceptualization. **A. Magni:** Software, Methodology. **M. Mastrogiovanni:** Software, Investigation. **L. Luzzi:** Supervision, Funding acquisition, Conceptualization. **D. Pizzocri:** Writing – review & editing, Methodology, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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