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Integral-scale validation of the SCIANTIX code for Light Water Reactor fuel rods

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ABSTRACT

Mechanistic multi-scale modelling holds the potential to inform fuel performance codes by incorporating high-fidelity models, algorithms, parameters, and material properties. In this context, meso-scale codes emerge as valuable tools for developing detailed models and performing separate verification and validation steps. This work focuses on SCIANTIX, an open-source 0D meso-scale code designed to describe the behaviour of gaseous and volatile fission products in nuclear oxide fuel. The code predominantly employs engineering physics-based behavioural models featuring computational times that align with typical fuel performance code requirements. Given the numerical foundation of the code, it is applicable to both stationary and transient conditions. Following a recent work outlining the standalone SCIANTIX (version 2.0) performance and its separate-effect validation database, we present its performance when coupled with fuel performance codes to simulate light water reactor fuel rods. The experiments selected for the comparative analysis constitute an initial integral validation database. The comparison focuses on conventional engineering quantities of interest, such as integral fission gas release, demonstrating the satisfactory performance of the code. Additionally, it highlights the potential advantages of multi-scale modelling over conventional semi-empirical approaches.

1. Introduction

Currently, several research efforts for Light Water Reactors (LWRs) target the development and improvement of methodologies and simulation tools for fuel rod performance analysis (e.g., within the Euratom Horizon 2020 Project R2CA and Horizon Europe Project OperaHPC). Material behaviour modelling plays a crucial role in complementing these advancements, and the developed Fuel Performance Codes (FPCs) serve as valuable toolsto model, predict, and interpret fuel rod behaviour. A comprehensive characterisation of fuel rod changes during irradiation under any circumstance is challenging due to the harsh core environment, so most existing data either address similar conditions or provide integral variables to compare with. Consequently, most engineering codes adopt semi-empirical approaches [1–3]. For this reason, conventional models and tools present some limitations regarding predictive capabilities when applied to different operational conditions or materials, delaying improvements of current LWRs regarding flexibility and safety. Furthermore, the qualification of an industrial (and proprietary) code is a long process that can potentially require time frames that are not perfectly in line with current scientific advances, where interesting developments in modelling, numerical methods, machine learning, and data-driven techniques are constantly emerging. [4–7]. The primary obstacle stems from outdated programming functional logic, slowing modular integrations—for instance, adopting a different (verified) numerical solver implies modifications in multiple subroutines. Mechanistic multi-scale modelling approaches hold the potential to inform FPCs by incorporating high-fidelity models and material properties [8,9], as well as improved numerical algorithms [10–12]. In this context, meso-scale codes emerged as valuable tools for developing detailed models and conducting separate verification and validation steps [13,14]. Therefore, the surgical integration of (verified and validated) meso-scale codes into integral codes accelerates and extends their predictive capabilities, providing a robust physical ground derived from lower-length experiments [15] and atomistic-scale simulations [8,9,16].

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In this work, we use the 0D open-source meso-scale code SCIANTIX (version 2.0), designed to describe Fission Gas Behaviour (FGB) with engineering and physics-based models [13,17]. The 0D approach adopted in the code means that the fuel grain domain is not discretised. In particular, the fission gas behaviour problem is solved over an ideal spherical fuel grain. The diffusion-decay equation (the only partial differential equation currently in the code) is expanded over a finite number of eigenfunctions of the spherical Laplacian operator [10–12]. Therefore, intra-granular gas concentrations and other important intra- and inter-granular quantities (e.g., bubble density, gaseous swelling, etc.) are calculated as average quantities in the spherical fuel grain. Several novelties of interest in FPCs have been introduced in the latest 2.0 version of the code [17]. Besides the computation of Fission Gases (FGs) xenon and krypton, and intra/inter-granular bubble concentrations [13,18,19], the code considers helium behaviour [20,21], radioactive isotopes [22,23], and peculiar microstructural processes related to High-Burnup Structure (HBS) formation and evolution [24,25]. Beyond these advancements, SCIANTIX 2.0 introduces a versatile framework that paves the way for the application to a broader spectrum of fission products, including volatile Fission Products (FPs), iodine, caesium, and tellurium,[1] as well as innovative nuclear materials (e.g., advanced technological fuels with specific dopants [28,29]).

The code is usable as a standalone program to develop and test detailed physics-based models and numerical solvers with corresponding verification and separate-effect validation steps. Notably, the use of SCIANTIX coupled with thermomechanical FPCs allows performing calculations of the quantity of engineering interest (e.g., by calculations of the integral Fission Gas Release (FGR)), with a better understanding of the underlying fundamental physical phenomena. SCIANTIX has been successfully coupled with several conventional and modern FPCs, working as a physics-based alternative to the standard FGB models [30–32]. Through this approach, the meso-scale code holds the potential to inform FPCs that rely on correlation-based approaches [33–35] to address the FGB problem. The separate-effect validation of the code ensured the accuracy of each implemented model [17].

Given the lack of a corresponding integral validation database, hindering the use of SCIANTIX at the industrial and design level, this work aims to present the first comprehensive integral validation database in LWR fuel rod conditions. Since the integral validation of the meso-scale SCIANTIX code requires the typical FPC infrastructure, we exploit the couplings with and TRANSURANUS [23,36], FRAPCON/FRAPTRAN [37], and OFFBEAT [38]. The validation database for LWR fuel herein considered encompasses 42 rods, covering different reactor operating conditions and burnup ranges. SCIANTIX predictions are assessed against experimental data, including thermal behaviour and fission gas release calculated during base irradiation and power ramps.

The outline of this work follows. Section 2 summarises the current SCIANTIX 2.0 integral couplings. Section 3 illustrates the simulated integral irradiation experiments. Section 4 discusses the obtained results, and Section 5 draws conclusions and discusses future developments.

2. The fuel performance codes coupled with SCIANTIX

This section summarises the features of SCIANTIX 2.0 and illustrates current couplings with integral thermomechanical FPCs.

2.1. SCIANTIX meso-scale capabilities, numerical and modelling features

SCIANTIX (version 2.0) is an open-source meso-scale code designed to model the behaviour of FGs/FPs of interest in nuclear oxide fuel. The code predominately employs physics-based models built on kinetic rate-theory descriptions. While retaining a level of complexity suitable for application to engineering fuel rod scale and consistent with the uncertainties about some parameters [39], the models describe fundamental physical processes such as gas atom diffusion and precipitation, gas bubble nucleation, growth, and formation of a percolation path. FGR and gaseous swelling are modelled as inherently coupled. Also, the models capture rapid release kinetics (burst release) observed during transients [40–42]. The implemented Ordinary Differential Equations (ODEs) are solved with first-order implicit schemes, with all the numerical solvers rigorously verified by the Method of Manufactured Solutions (MMS) method. Therefore, the computational effort required by a single SCIANTIX call is limited to a few milliseconds, yet it provides accurate numerical solutions. The system of ODEs implemented in the code consists of non-linear coupled differential equations. To keep execution times short and provide a light computational burden to engineering FPC, we adopted the operator-splitting method as a linearisation strategy [43].

2.2. Coupling with fuel performance codes

Meso-scale codes have the great advantage of rapidly extending the predictive capabilities of FPCs by including new (separately-validated) model improvements and avoiding significant modification of the source code.[2] Considering the low computational times of each SCIANTIX execution, the most effective coupling strategy involves the *online coupling*. This entails a continuous data transfer between the two systems directly within the computer memory during the main program execution.[3]

In the considered fuel rod performance analysis, the integral FPCs perform thermomechanical calculations in each quadrature point of discretisation element on the fuel rod geometry. In each of these points, the FPCs execute the meso-scale code SCIANTIX 2.0 to retrieve a set of local quantities of interest (e.g., FG concentrations and gaseous swelling) from thermo-mechanical variables such as local temperature and fuel hydrostatic stress.

As for the execution time of SCIANTIX coupled with integral codes, there is an expected increase in the simulation time. The computation time of TRANSURANUS, FRAPCON, and OFFBEAT is doubled/tripled depending on the case. Such a time increase may be somehow less critical with fast-running codes (i.e., TRANSURANUS and FRAPCON). On the other hand, further optimizing CPU management is a high priority to minimize computational time. Along with the increased computational time, there is an improvement in the thermo-mechanical iterative scheme at the same convergence limit due to the numerical solutions of SCIANTIX 2.0, bounded in terms of numerical error [10,13].

2.2.1. TRANSURANUS

TRANSURANUS is a 1.5-D FPC, representing the fuel rod geometry with an axisymmetric, axially stacked, 1-D radial representation. The fuel rod is discretised in axial slices, or sections, in radial coarse zones to evaluate the material properties and in finer zones to perform the numerical calculations. For FGB analysis, TRANSURANUS relies on the recommended semi-empirical model [30–32]. A more mechanistic treatment is also available, based on the work of Pastore et al. [18], but since this choice is not yet recommended as it is still subject to review, we focus on the recommended model. When coupled with SCIANTIX 2.0, FGB related variables are calculated by the meso-scale code. The coupling of the codes is supported via a specific binding interface, which provides communication between TRANSURANUS (Fortran) and SCIANTIX 2.0 (C++).

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[1] Such modelling will require the inclusion of oxidation/reduction steps between UO_2 and FPs, based on thermochemical equilibrium calculations [26,27]. To maintain a low computational time in line with engineering FPC applications, surrogate modelling techniques applied to thermochemical databases are of potential interest.

[2] This feature is of great interest when proprietary codes and tools with limited access to the source code are involved.

[3] From a practical point of view, such communication can be set up via proper binding interfaces that ensure variable conversion (e.g., from Fortran to C++ and vice versa) without loss of data [23] [44].

2.2.2. *FRAPCON and FRAPTRAN*

FRAPCON and FRAPTRAN are also 1.5-D FPC, with a geometrical fuel rod representation similar to the TRANSURANUS one. Namely, these codes operate an axisymmetric, 1-D radial fuel rod analysis. The fuel rod is axial discretised, with double radial discretisation for the fuel pellet: one for the thermomechanical problem and one for the fission gas calculation. Most of the implemented material (e.g., fuel and cladding) properties and correlations are taken from the MATPRO library [45]. As for the FGB analysis, FRAPCON relies on the best-estimate semi-empirical model recommended by Pacific Northwest National Laboratory (PNNL) [30,31]. Other possibilities are available: the ANS-5.4 fission gas release model [46] and the FRAPFGR model. The latter is based on a modified version of the previous recommended model, and it is used mainly for initialising the FRAPTRAN transient FGR model before simulations of accidents (e.g., during Reactivity-Initiated Accidents (RIAs)). Both FRAPCON and FRAPTRAN have been recently coupled with SCIANTIX in the frame of the H2020 R2CA European Project. When coupled with SCIANTIX, quantities related to FGB are calculated by the meso-scale code. The coupling of the codes is supported via a specific binding interface, providing the FRAP (Fortran) and SCIANTIX (C++) communication.

2.2.3. *OFFBEAT*

The OFFBEAT code is a recently developed open-source multi-dimensional FPC [38,47,48]. The code is usable for the 1.5, 2 and 3-D analysis of the fuel rod. The code adopts the finite volume method to solve the governing thermo-mechanical problem. The OFFBEAT code was assessed in LWR conditions but is currently under development (and further assessment) along several lines of research, e.g., Mixed Oxides (MOX) and TRISO fuel. Concerning LWR fuel rod, most of the material properties for fuel and cladding behaviour are based on the MATPRO library [45]. Currently, OFFBEAT is equipped with SCIANTIX as FGB model, with a direct online coupling eased by the common C++ framework.

3. Integral-scale validation

The validation process[4] is an essential step to check the robustness and the reliability of a code [49]. Also, for developers, it is often a meaningful way to check whether the code captures the response of the system with a required accuracy. The content of this section concerns the validation of the SCIANTIX code when used at the engineering integral scale, aiming at assessing the predictive capability when applied to simulations of nuclear fuel rods irradiated in LWR conditions.

3.1. *Data sources and criteria for comparison*

The experimental database forms the backbone of the validation process. Hence, it is essential to include different fuel rod irradiation conditions in different scenarios. Experimental data obtained from various sources, including in-pile experiments and post-irradiation examinations, serve as a reference for the validation. The considered dataset encompasses experiments from the International Fuel Performance Experiments (IFPE) database [53], including fuel rods irradiated at different burnup levels and under various operational conditions, ensuring a robust examination of the SCIANTIX calculations.

Table 1
Validation matrix illustrating the FPCs coupled with SCIANTIX 2.0, used to carry out the integral validation, and the simulated experimental cases.

Experiment	Rod	TRANURANUS	FRAPCON	FRAPTRAN	OFFBEAT
IFA-432	1,3,5				X
IFA-562	1:12				X
IFA-650	9			X	
IFA-650	10	X		X	
CONTACT	1	X			X
HATAC	C2	X	X		X
Risø-3	AN3	X	X		X
REGATE		X	X		X
SUPERRAMP	PK series	X			X
SUPERRAMP	PW series	X			X
SUPERRAMP	BK series	X			X

The accurate prediction of the thermo-mechanical response depends mainly on the code ability to capture the high burnup effect, fuel swelling, FGR, cladding creep-down, fuel thermal conductivity degradation, and fuel-cladding gap behaviour. The validation criteria selected for this work include quantitative metrics for FGR, related to xenon and krypton concentrations, and Fuel Central Temperature (FCT). The criteria are established based on conventional standards, ensuring a consistent assessment of the code performance against integral-scale experimental data. Ultimately, the validation process highlights SCIANTIX 2.0 strengths and identifies areas for potential improvement, contributing to code refinement for future applications.

Comprehensive validation campaigns have been carried out for several FPCs, e.g. FRAPCON [54], TRANSURANUS [55] or BISON [56]. The focus is on integral measurements, intrinsically 1-D if not 0-D (e.g., FCT, the gap pressure and the rod free volume, the cladding elongation, and the FGR).

The primary efforts carried out as part of the work are presented in this section and are focused exclusively on the FCT and FGR fractions for several rods from the IFPE database. The experiments reproduced with SCIANTIX 2.0 coupled with FPCs are presented in Table 1 and discussed later in more detail.

3.2. *Modelling choices*

The following sections illustrate the performance of FRAPCON, TRANSURANUS and OFFBEAT coupled with SCIANTIX (version 2.0) applied to the simulation of LWR fuel rods. Specifically, the validation database encompasses fuel rods operated in stationary and transient conditions [53]. Since SCIANTIX is a physics-based meso-scale code, no *a priori* calibration is applied, and the implemented UO_2 properties are expressed according to their reference values. The intra-granular gas and bubble behaviour models describe the xenon and krypton intra-granular diffusion, trapping and irradiation-induced re-solution and gas bubble nucleation outlined in the work of Pizzocri et al. [57]. The inter-granular gas and bubble behaviour models consider the gas accumulation at the grain boundaries and the evolution of the gas bubbles following bubble growth, coalescence and interconnection. The grain-boundary bubble evolution is driven by the vacancy inflow/outflow according to Speight and Beere approach [58], with the vacancy diffusivity formulation derived in the work of White [40]. The onset for thermal FGR is taken from the work of Pastore et al. [18], modelling the thermal release after reaching a fixed threshold of the grain-boundary fractional coverage. In base-irradiation conditions, the burst release model due to grain-boundary micro-cracking is not considered. The main reason for this choice is that the burst release model was built following separate-effect experimental data that experienced abrupt temperature transients [19]. Conversely, this model is activated only during transient conditions, where the burst release of fission gas was experimentally observed. The adopted FGB model settings are listed in Table 2.

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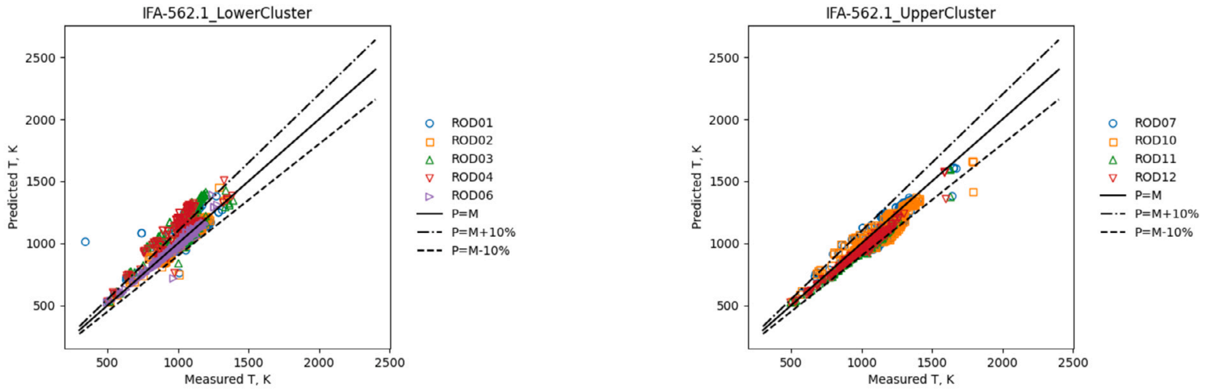
[4] Another fundamental step for the code qualification process, namely, the verification, is considered a prerequisite to the validation. Verification assesses the predictions of the code against analytic solutions. It is particularly relevant because the compensation of errors of a numerical nature may hinder fundamental issues from incorrect numerical/implementation schemes. Because of the new SCIANTIX 2.0 code architecture, i.e., with independent classes for models and solvers, the code verification is performed via MMS [50,51] and is available at the online code repository [17,52].

Table 2
Model settings adopted in SCIANTIX 2.0 coupled with integral FPCs for LWR fuel rod simulation.

Model	Form	Condition	Reference
Grain growth	Ainscough et al. model	Base, transient	[59]
D, xenon single-atom diffusivity	$D = D_1 + D_2 + D_3$ $D_1 = 7.6 \times 10^{-10} \exp(-4.86 \times 10^{-19}/k_B T)$ $D_2 = 5.64 \times 10^{-25} \sqrt{\dot{F}} \exp(-1.91 \times 10^{-19}/k_B T)$ $D_3 = 8 \times 10^{-40} \dot{F}$	Base, transient	[60]
g, trapping rate	$g = 4\pi D(R_{ig} + R_{sg}) N_{ig}$	Base, transient	[61]
b, resolution rate	$b = 2\pi \mu_{ff}(R_{ff} + R_{ig})^2$	Base, transient	[62]
D_v, grain-boundary vacancy diffusivity	$D_v = (3.5/5) 8.86 \times 10^{-6} \exp(-4.17 \times 10^4/T)$	Base, transient	[40]
Grain-boundary micro-cracking	Barani et al. model	Transient	[19]



(a) Predicted vs. measured temperature for rods 1, 2, 3, 4 and 6 of the IFA-562 (lower cluster) bundle.

(b) Predicted vs. measured temperature for Rods 7, 10, 11 and 12 of the IFA-562 (upper cluster) bundle.

Fig. 1. Predicted vs. measured temperature for rods of the IFA-562 bundle. Calculations are performed with OFFBEAT coupled with SCIANTIX 2.0.

3.3. IFA-432 and IFA-562

Although this work mainly emphasises validating the meso-scale code SCIANTIX 2.0 for FGR prediction, assessing fuel temperature predictions with experimental data is essential. This is crucial because the local fuel temperature plays a dominant role in fuel performance, safety analysis, and all critical phenomena occurring within fuel rods, with an essential intrinsic connection between FGR and local fuel temperature [39,63]. Also, it is necessary for the OFFBEAT code given that SCIANTIX is the only default FGB model.

Numerous experiments have been conducted with local measurements of the FCT using either a thermocouple or extensometer. Available rods from IFA-432 and IFA-562 bundles are used to assess the thermal performance of OFFBEAT coupled with SCIANTIX 2.0. The IFA-562.1 consisted of 12 instrumented rods, irradiated in the Halden Boiling Water Reactor (HBWR) up to a burnup of 10 MWd kgU^{-1}. The rods were equally divided between a lower and an upper cluster of 6 rods fabricated by two manufacturers. Each cluster contained a pair of rods filled with helium, while others were filled with xenon. All rods were instrumented with thermocouples and extensometers. To better isolate the effect of surface roughness, the rods were fabricated with a small initial gap to favour gap closure. They were irradiated at low power to limit fission gas release. A short ramp followed the base irradiation to investigate the fuel grain growth during power transients.

Figs. 1a, 1b and 2 illustrate the calculated FCT for IFAs listed in Table 1. In particular, IFA-562 (Figs. 1b and 1a) is representative of low-burnup fuel (10 MWd kgU^{-1}), while IFA-432 (Fig. 2) for medium-burnup fuel (32 MWd kgU^{-1}). Two added dashed lines correspond to a ±10% relative error. Considering the state-of-the-art uncertainty range for the calculated fuel temperature (i.e., 10% at a confidence level of 95%), the comparison between measured and predicted fuel temperature is satisfactory for OFFBEAT coupled with SCIANTIX 2.0, considering traditional sources of uncertainties (e.g., exact thermocouple position, fresh fuel characterisation, uncertainty range for fuel parameters, etc.), and comparison with other FPCs (e.g., BISON [56]). Also other rods (e.g., CONTACT1 and Risø-3 AN3) are used to re-assess or validate FCT calculations among several FPCs coupled with SCIANTIX.

3.4. Super-Ramp

This section briefly summarises the FGR predicted with TRANSURANUS and OFFBEAT coupled with SCIANTIX 2.0 for a subset of fuel rods from the Super-Ramp program [64]

3.4.1. Experiment description

The Studsvik Super-Ramp project, included in the IFPE database, aimed to investigate the behaviour of LWR fuel rods during power ramps. The program comprised fuel rods with several designs, base-irradiated and then power-ramped. In this work, the focus is on 18 rods from the Pressurized Water Reactor (PWR) subprogram (PK1, PK2, PK4, PK6, PW3) and 4 rods from the Boiling Water Reactor (BWR) subprogram (BK7).

PK1 and PK2 consisted of standard fuel rods that successfully withstood power ramping despite experiencing significant deformations and FGR. PK6 rods had a larger grain size, resulting in lower FGR than PK1 and PK2. One rod, PK1-6, failed, revealing substantial fuel-to-clad bonding through Post-Irradiation Examination (PIE).

3.4.2. Simulation results

The comparison between the integral FGR calculated at the end of irradiation and the measured values is illustrated in Fig. 3. The calculated integral FGR demonstrates a satisfactory comparison, providing accurate predictions for most rods. This is particularly noteworthy given the typical deviations observed in the literature, with the two dashed lines in the figure representing deviations of a factor of 2 from measured data.

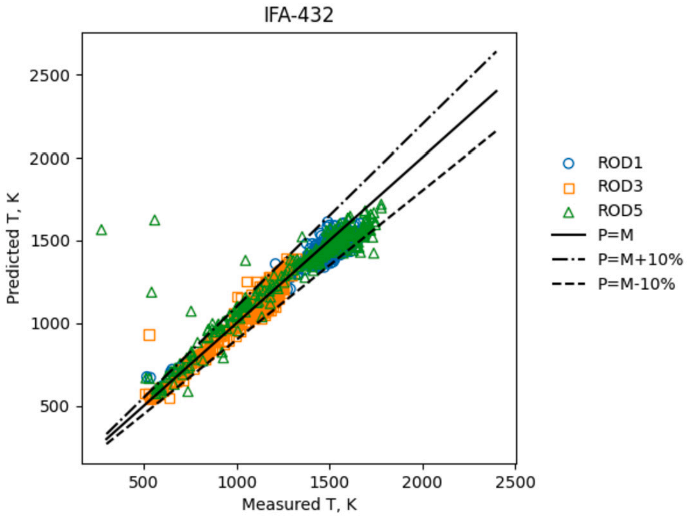


Fig. 2. Predicted vs. measured temperature for rods 1, 3 and 5 of the IFA-432 bundle. Calculations are performed with OFFBEAT coupled with SCIANTIX 2.0.

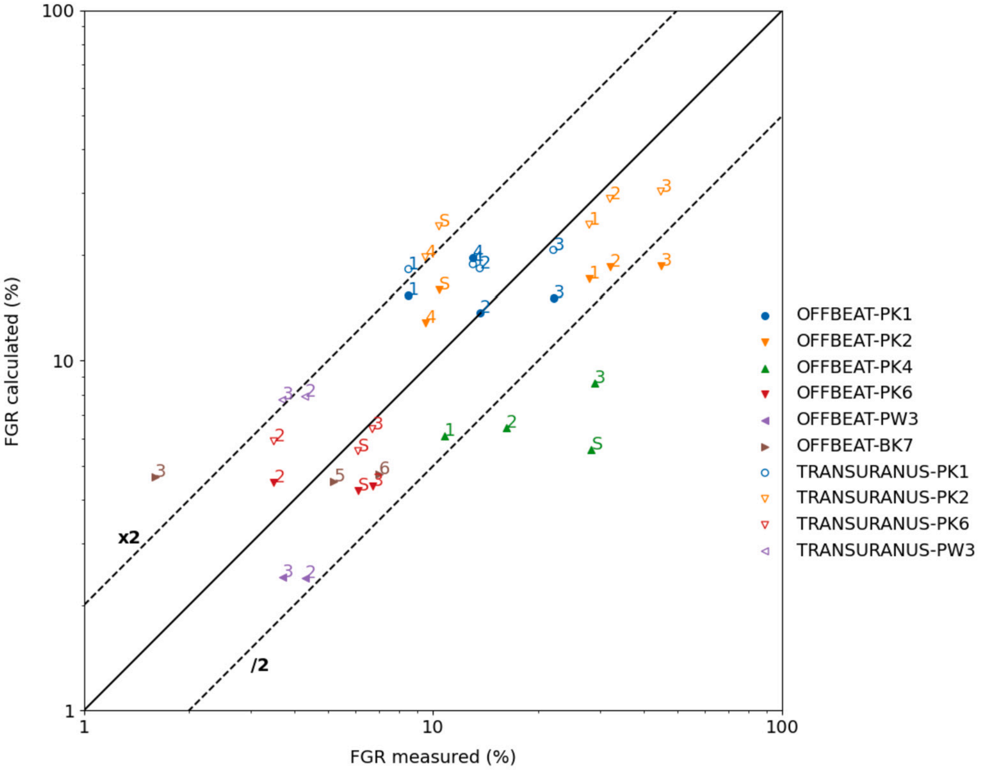


Fig. 3. Super-Ramp: Fission gas release. The symbols represent the integral fission gas released measured and calculated at the end of the considered Super-Ramp simulated rods.

3.5. Risø-3 AN3

3.5.1. Experiment description

The Risø-3 program consisted of bump-tests to investigate FGR and microstructural changes of several refabricated and re-instrumented fuel rods. The behaviour of such fuel rods has been extensively analysed and employed to validate several FPCs, e.g., the BISON code [56], the COSMOS code [65,66], and also separate FGB model [19,67,68]. The segment AN3 was base-irradiated in the Biblis A PWR (Germany, 1982-1986) up to a final burnup of approximately 41.8 MWd kgU^{-1} before being bump-tested for 72 hours in the test reactor DR3 (Risø, Denmark) under PWR conditions. The AN3 rod was refabricated before the bump test and purged of the FG released during the base irradiation. The fuel segment was shortened, drilled at the top and loaded with helium at 14.7 bar. The refabricated fuel segment was instrumented with a pressure transducer and a thermocouple to measure the local fuel temperature at 1.5 pellet heights above the bottom of the thermocouple hole. After the entire bump test, reaching a peak power of about 40 kW/m, the segment was punctured, and the total FGR was measured.

3.5.2. Simulation results

Fig. 4 illustrates the difference between the measured and calculated FCT during the bump test of the rod AN3. The results provided by the codes agree with the thermocouple measurement and are consistent with each other. The inherent differences in the temperature predictions

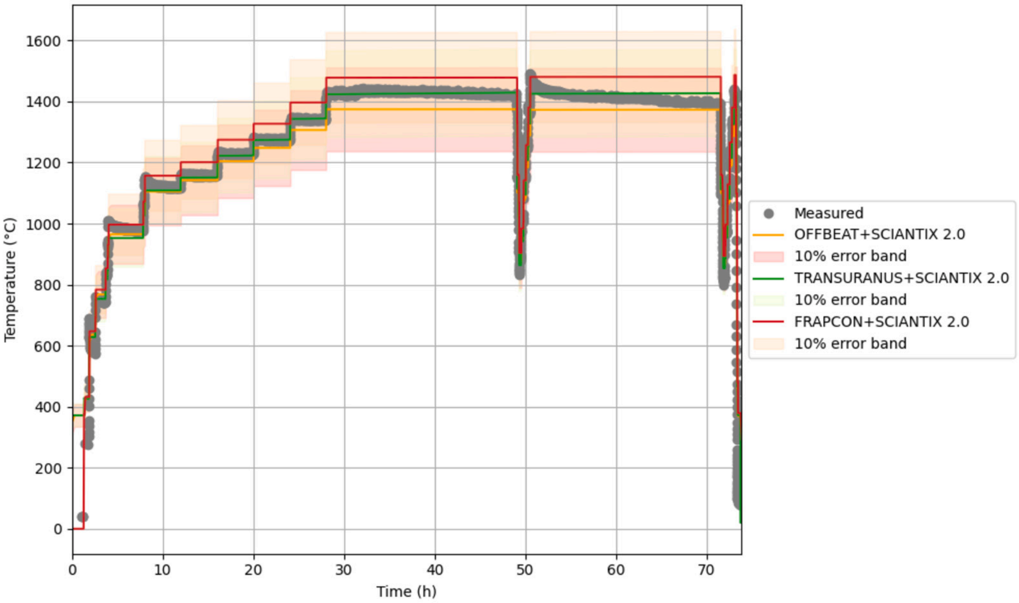


Fig. 4. AN3 - Bump test: Fuel temperature. Grey points represent the fuel temperature measured by the thermocouple. Solid lines are calculated with FPCs coupled with SCIANTIX 2.0, namely, OFFBEAT (orange line), TRANSURANUS (green line), and FRAPCON (red line). The filled regions represent deviations from the considered code calculations of 10%. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

are explainable by intrinsic code differences and common modelling assumptions when simulating base irradiation followed by refabrication (shortened rod geometry for the base irradiation and approximations involved in simulating the rod refabrication process). Nevertheless, measured fuel temperatures fall within the uncertainty range of about 10% from the code calculations. Also, for the sake of readability, the temperature predicted by standalone TRANSURANUS and FRAPCON are not displayed in Fig. 4 because calculations are almost superposed to the calculations of the codes coupled with SCIANTIX 2.0. The central temperature values are mostly affected by the axial power profile and the central hole for the thermocouple. The three FPCs show discrepancies in the predicted temperature behaviour after the power ramp. Indeed, the experimental temperature slightly decreases while code calculations remain flat. This was a common behaviour observed in the Coordinated Research Project on Fuel Modelling at Extended Burnup (FUMEX-II) [69], highlighting a possible contribution of the fuel creep that could cause the pellet to expand after each sudden power increase, decreasing the gap-width and the fuel temperature.

As for FGB, in LWR base-irradiation conditions, low values of FGR (<1-2%) are generally observed [2]. Low values of the calculated FGR exhibit substantial variation factors, while calculated values for large FGR (> 15%) are characterised by a deviation factor of about 2 [39]. This behaviour is supposably driven by intrinsic uncertainties in modelling the onset of thermal diffusional FGR, which is a dominant contribution. Therefore, nuclear FPCs tend to employ mostly empirical or semi-empirical approaches to estimate the FGR in nominal reactor conditions. Fig. 5a illustrates the FGR calculated with the considered codes during the AN3 base irradiation, compared to the experimental value obtained at the end of the base irradiation from the puncturing test. The three codes (TRANSURANUS, FRAPCON, OFFBEAT) coupled with SCIANTIX, predict reasonable FGR values: 0.66%, 0.5%, and 0.36%, respectively. These results also align with the default TRANSURANUS and FRAPCON values, predicting 0.28% and 0.26% of FGR against the measured value of 0.2%.

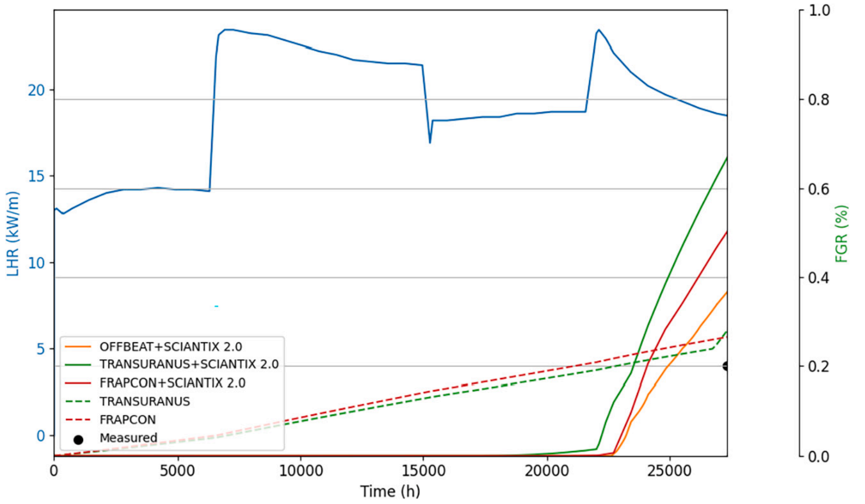
The Risø-3 AN3 bump test calculations are illustrated in Fig. 5b. The release kinetics during the first 50 hours of the bump test is satisfactorily represented: the experimental FGR increases by about 15%, starting from 5% (at 10 hours) up to 20% (at 50 hours). The three codes that use SCIANTIX predict in the same temporal range a transient FGR in the interval 5-11%. During the first 50 hours of the bump test, the release calculated with SCIANTIX is mainly a thermal-driven contribution from gas accumulated in grain-boundary gas bubbles. Afterwards, the release calculated by the three codes coupled with SCIANTIX from 50 hours to the end of the test is largely due to a-thermal gas release mechanisms due to grain-boundary micro-cracking events. At the end of the irradiation, these calculated gas release values are in the range of 15-18%. The transient FGR measured during the bump test is notably underpredicted. Such underprediction is common in state-of-the-art calculations and indicates a lack of burst fission gas release descriptions. Regarding the SCIANTIX code and the present analysis, because of the uncertainties involved in FGB modelling and the common FPC calculations, the predictive accuracy remains satisfactory (see Table 5). Nevertheless, efforts towards an improvement in grain-boundary micro-cracking modelling have to be undertaken, possibly combining SCIANTIX calculations of the grain-face bubble pressure with the local stress field near grain-face bubbles that could lead to micro-cracking events [70]. As for the gas release predicted by TRANSURANUS and FRAPCON, their calculations show a similar behaviour since their own FGR calculations follow the description developed in [31,30]. The major differences result from the effective xenon diffusion coefficients, with TRANSURANUS employing the Matzke correlation [71], and FRAPCON using a different calibrated correlation.

3.6. CONTACT1

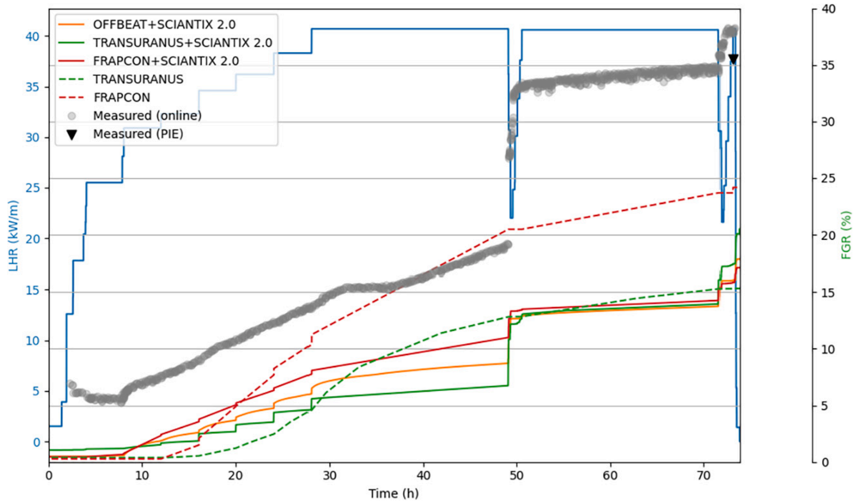
In this section, the FPCs TRANSURANUS and OFFBEAT coupled with SCIANTIX 2.0, and standalone TRANSURANUS are applied to the simulation of the CONTACT1 experiment.

3.6.1. Experiment description

The CONTACT1 experiment took place in the SILOE reactor, in which a short fuel rod with five UO_2 pellets (for a total height of 7 cm) with a Zr-4 cladding was irradiated up to burnup values of about 22 MWd kgU^{-1}. The rodlet was located in a PWR loop, at 13 MPa, with a cladding temperature of 330°C. The LHR (of about 40 kW m^{-1}) was measured by rhodium neutron detectors with an accuracy on the measurement of 3%. The neutron flux was substantially uniform, the axial power variations negligible, i.e., less than 2% [72]. The experimental rod had a FCT



(a) AN3 - Base irradiation: Fission gas release. The black dot represents the measured fission gas release. The solid lines are the calculations of the considered FPCs coupled with SCIANTIX 2.0: OFFBEAT (orange line), TRANSURANUS (green line), and FRAPCON (red line). The dotted lines are the default calculations of the considered FPCs: TRANSURANUS (green line) and FRAPCON (red line). The blue y-axis on the left is the Linear Heat Rate (LHR) imposed in the irradiation history.



(b) AN3 - Bump test: Fission gas release. The grey dots represent the fission gas release measured during the experiment (by rod internal pressure measurement). The solid lines are the calculations of the considered FPCs coupled with SCIANTIX 2.0: OFFBEAT (orange line), TRANSURANUS (green line), and FRAPCON (red line). The dotted lines are the default calculations of the considered FPCs: TRANSURANUS (green line) and FRAPCON (red line). The blue y-axis on the left is the LHR imposed in the irradiation history.

Fig. 5. Results of the AN3 fuel rod simulation. Calculations are performed with TRANSURANUS, OFFBEAT, and FRAPCON, coupled with SCIANTIX 2.0., and standard TRANSURANUS and FRAPCON.

measurement probe accommodated in a 1.5 mm diameter central annulus and gas lines to sweep the fission gas released during irradiation. The irradiation experiment proceeded for 11 cycles. Each irradiation cycle consisted of 21 days of irradiation per month. The shutdown at 8 MWd kgU^{-1} was forced by the accidental introduction of air into the water loop, which caused the fuel rod to experience a shock wave without any deterioration of the instrumentation. From the beginning of the irradiation up to the shutdown at 8 MWd kgU^{-1}, the rod internal pressure was imposed at a value of 1 MPa, with helium as sweeping gas. After the shutdown until the end of the irradiation, the rod internal pressure was imposed at 0.1 MPa, with neon as sweeping gas. Such a gap environment must be considered to estimate correctly the fuel temperature. [72]. Other details are collected in Table 3. The considered results concern the evolution of FCT, fractional release of stable fission gas (obtained through the measurement of the long-lived ^{85}Kr isotope) and release-to-birth ratio of short-lived fission gases.

3.6.2. Simulation results

OFFBEAT, TRANSURANUS coupled with SCIANTIX 2.0, and standalone TRANSURANUS are employed to simulate the CONTACT1 irradiation experiment and extract code calculations in terms of FCT, FGR, and release-to-birth ratio. Assessing the thermal performance of the codes, Fig. 6 illustrates the imposed LHR, with the measured and calculated FCT. The agreement of OFFBEAT and TRANSURANUS (standalone and with SCIANTIX 2.0) with the experimental data is reasonable; code predictions in terms of temperature are well enclosed in the 10% uncertainty range, suitable for fuel temperature calculations [39].

As for the analysis of the FGB, simulation results are shown in Fig. 7a. TRANSURANUS and OFFBEAT coupled with SCIANTIX 2.0 predict a similar FGR, with also a release kinetics similar to the experimental one. The calculated FGR at the end of the irradiation is about 14.4% for OFFBEAT using SCIANTIX 2.0 and 16% for TRANSURANUS with SCIANTIX 2.0, with an experimental value of 18.4%. The default TRANSURANUS

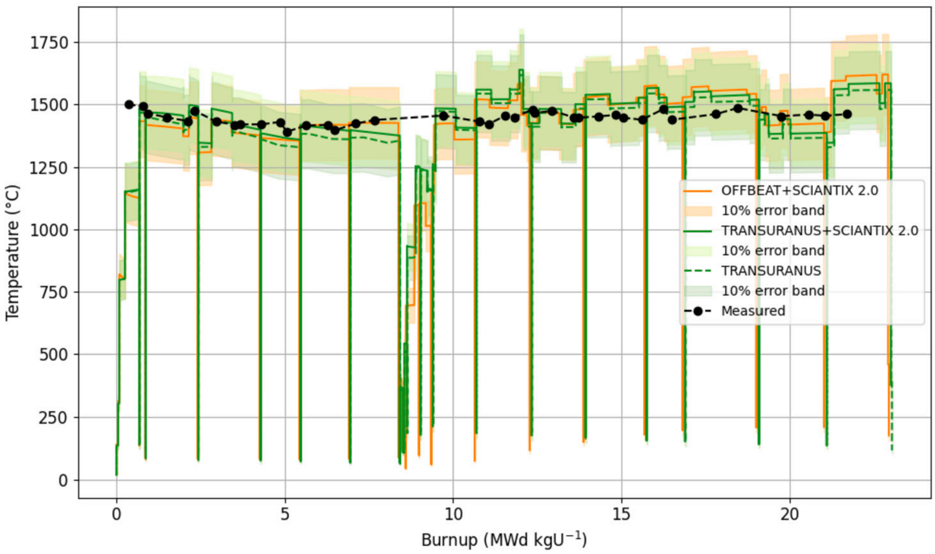


Fig. 6. CONTACT1: Fuel temperature. Black dots are experimental measurements connected by dotted lines to improve readability. The green solid line is calculated with TRANSURANUS and SCIANTIX 2.0, the orange solid line is calculated with OFFBEAT and SCIANTIX 2.0, the green dotted line is calculated with the standard TRANSURANUS code. The filled regions represent deviations from the considered code calculations of 10%.

Table 3
Design data of the CONTACT1 fuel rod [72,73].

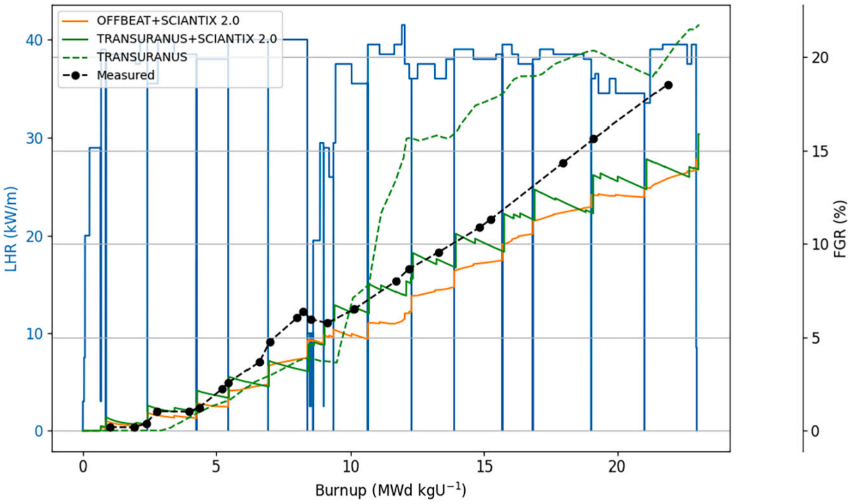
	Parameter	
Fuel pellets	Height (mm)	14
	Diameter (mm)	8.19
	Dish depth (mm)	0.13
	Dish radius (mm)	14.73
	Central TC hole (mm)	0.75
Cladding	Internal diameter (mm)	8.36
Cladding	External diameter (mm)	9.50
Plenum	Height (mm)	7.7
	He, pressure before shutdown (MPa)	1
	Ne, pressure after shutdown (MPa)	0.1
Fuel column	Number of pellets	5
	Enrichment (%)	4.95
	Theoretical density (%)	95
Irradiation	Nominal rating (kWm^{-1})	40.5
	Peak rating (kWm^{-1})	41
	Average rating (kWm^{-1})	36
	Fast flux ($E > 1$ MeV) (m^{-2} s^{-1})	6.5×10^{17}
	Discharge burn-up (MWd kgU^{-1})	22
	Clad ext. temperature (°C)	330
System pressure (MPa)		13

version predicts a different release kinetic, with a final FGR of about 21.6%. Overall, all the code calculations reasonably agree with the experimental data. The use of SCIANTIX as a physics-based FGB module is a promising alternative to the adopted empirical models, with a satisfactory description of the FGR kinetics without increasing in a significant manner the computational times of the codes.

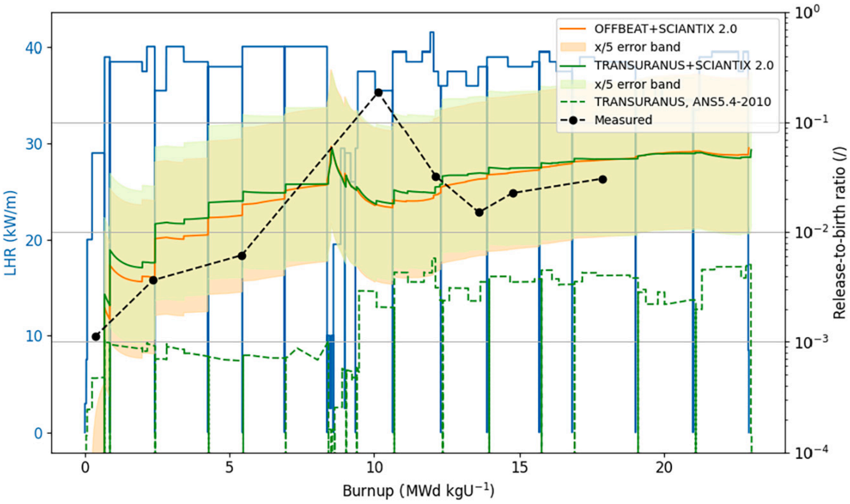
An additional analysis retrieved from the CONTACT1 simulation is the evaluation of the radioactive gas released from the fuel and accumulated in the fuel-rod-free volume. To evaluate the gap activity, conventional FPCs may employ semi-empirical approaches or fixed thresholds, quantifying the radioactive FG/FP release. Limitations may emerge when these methodologies are applied to accidental scenarios (e.g., Design-Basis Accident (DBA) and Design-Extended Condition - Type A (DEC-A) characterised by transient dynamics, which may result in potential excesses of conservatism. In this regard, the multi-scale coupling with physics-based meso-scale codes demonstrates its potential. Specifically, SCIANTIX 2.0 includes physics-based models for radioactive FGs in UO_2, with an intra-granular radioactive formulation for the isotopes available as single-atoms and trapped within intra-granular bubbles and a subsequent description for their accumulation/decay at grain-boundary bubbles. The integral FPCs also benefit from the numerical capabilities of SCIANTIX 2.0, adopting the extended Spectral Diffusion Algorithm (SDA) to solve the time-dependent diffusion-decay intra-granular problem, with controlled numerical errors [11]. This approach can overcome current semi-empirical approaches based on the equilibrium solution of the diffusion-decay problem [1], with a comprehensive intra-/inter-granular formulation built on a physics-based ground and verified numerical solvers. Eventually, the use of SCIANTIX is able to provide an acceptable representation of a large spectrum of short-lived radionuclides, which can be further adapted to specific needs or situations by using tuning parameters for the most relevant model parameters, that are, the gas and vacancy diffusivities, and the micro-cracking model parameters [10,19,22].

Fig. 7b shows the Release-to-Birth ratio (RB) of the short-lived ^{133}Xe (decay rate $\lambda = 1.53 \times 10^{-6}$ s^{-1}). The CONTACT1 experimental reports show no precise indication of the experimental R/B uncertainty. Because of the lack of an accepted uncertainty range for the calculated release-to-birth ratio, we consider a deviation on predicted/measured R/B calculations of about a factor of 5, as reported in the ANS 5.4-2010 report for IFA-504/558/633 calculations at burnup values of about 20 MWd/kgU [1] In Fig. 7b, the ^{133}Xe measurement at 10 MWd kgU^{-1} shows an unusual increase after the reactor shutdown, not reported for other radionuclides [22]. Such data points may be ascribed to instrumentation errors; in any case, such points must be cautiously considered and may not represent the gas thermal release.

The predicted R/B values are in satisfactory agreement with the experimental data and are consistent among TRANSURANUS and OFFBEAT. On the contrary, ANS 5.4-2010 underestimates the experimental R/B values. Eventually, SCIANTIX allows the use of fuel design parameters (e.g., fuel grain radius) to avoid any artificial calibration, yet with time-dependent predictions that agree with the experimental data. On the other hand, the semi-empirical ANS 5.4-2010 methodology considers a recalibration of two quantities in the computation of the release-to-birth ratios, namely, the intra-granular diffusivity D and the surface-to-volume ratio S/V, with substantial underestimation or deviation when applied to particular cases out of the validation database, as in the considered CONTACT1 case [22,23]. Such underestimation is noticeable in Fig. 7b.



(a) CONTACT1: Fission gas release. The green solid line is calculated with TRANSURANUS coupled with SCIANTIX 2.0, and the orange solid line is calculated with OFFBEAT coupled with SCIANTIX 2.0. The green dotted line is calculated using the standard TRANSURANUS code. The black circles are online measurements of ^{85}Kr fractional release, connected with dotted lines to enhance readability. The blue y-axis on the left is the LHR imposed in the irradiation history.



(b) CONTACT1: Release-to-birth ratio for the short-lived ^{133}Xe isotope. The green solid line is calculated with TRANSURANUS coupled with SCIANTIX 2.0, and the orange solid line is calculated with OFFBEAT coupled with SCIANTIX 2.0. The green dotted line results from the ANS 5.4-2010 methodology available in TRANSURANUS. The two filled areas correspond to a deviation from the code calculations of a factor 5. The black circles are online measurements of short-lived ^{133}Xe release-to-birth ratio, connected with dotted lines to enhance readability. The blue y-axis on the left is the LHR imposed in the irradiation history.

Fig. 7. Results of the CONTACT1 simulation. Calculations are performed with TRANSURANUS and OFFBEAT coupled with SCIANTIX 2.0 and with standard TRANSURANUS.

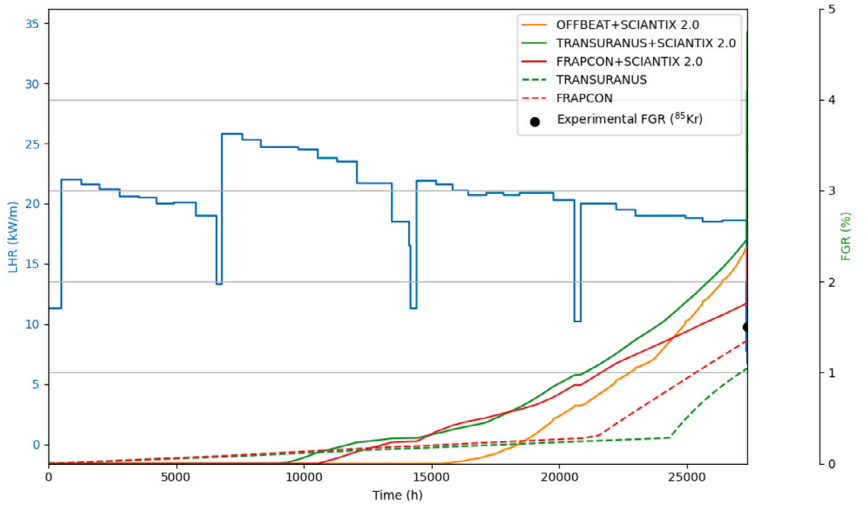
3.7. REGATE

3.7.1. Experiment description

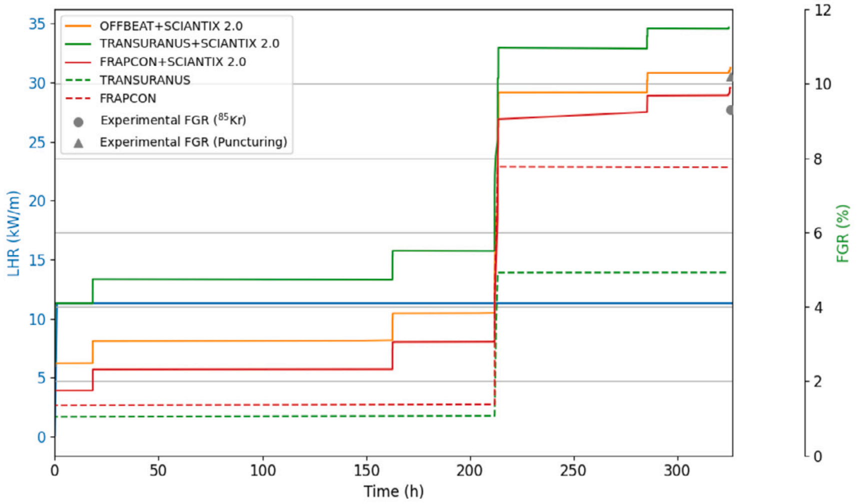
The REGATE experiment belongs to the Fuel Modeling at Extended Burnup (FUMEX-II) program [69] and to the IFPE database. The fuel rod that was considered for the experiment was a fuel segment irradiated in a commercial PWR (in-pile base irradiation in the Gravelines 5 PWR) and ramped in the French SILOE test reactor. The ramp test consisted of a pre-conditioning phase at 19.5 kW/m (peak power) for 48 hours before ramping at 1.0 kW/m/min up to 38.5 kW/m (peak power), held for 1.5 hours. The experiment provided data on FGR and clad diameter during power transient at medium burnup (47.415 MWd kgHM^{-1}). In particular, non-destructive PIE was performed on the fuel segment after discharge from the Gravlines 5 PWR with measurements on clad diameter and total FGR (based on long-lived ^{85}Kr gamma scan measurements). The total measured FGR after base irradiation was 1.5%. The fuel segment was not subject to any refabrication after base irradiation. After the ramp test in the SILOE reactor, the released ^{85}Kr was quantified via gamma scanning, and a total FGR of approximately 9.3% was obtained. Puncturing tests were also performed after the power ramp in the SILOE reactor to measure a total FGR of 10.2%.

3.7.2. Simulation description

The REGATE experiment has been simulated with TRANSURANUS, FRAPCON, and OFFBEAT, coupled with SCIANTIX 2.0. FGR calculations are reported in Fig. 8a, for the base-irradiation, and in Fig. 8b for the ramp test, together with the LHR. The fuel rod characteristics used for REGATE simulation are reported in the IFPE database and are available in the BISON validation database [56]. The modelling assumptions for the fuel rod simulations involve base irradiation fol-



(a) REGATE - Base irradiation: Fission gas release. The black dot represents the fission gas release measured at the end of the base irradiation via ^{85}Kr gamma scanning. The solid lines are the calculations of the considered FPCs coupled with SCIANTIX 2.0, namely, OFFBEAT (orange line), TRANSURANUS (green line), and FRAPCON (red line). The dotted lines are the default calculations of the considered FPCs: TRANSURANUS (green line) and FRAPCON (red line). The blue y-axis on the left is the LHR imposed in the irradiation history.



(b) REGATE - Ramp test: Fission gas release. The grey symbols represent the fission gas release calculated during the experiment: The grey triangle was derived from the ^{85}Kr gamma scanning, and the grey circle from the puncturing test. The solid lines are the calculations of the considered FPCs coupled with SCIANTIX 2.0, namely, OFFBEAT (orange line), TRANSURANUS (green line), and FRAPCON (red line). The dotted lines are the default calculations of the considered FPCs: TRANSURANUS (green line) and FRAPCON (red line). The blue y-axis on the left is the LHR imposed in the irradiation history.

Fig. 8. Results of the REGATE simulation. Calculations are performed with TRANSURANUS, FRAPCON, and OFFBEAT coupled with SCIANTIX 2.0 and with the standard TRANSURANUS and FRAPCON.

lowed by ramp irradiation (no refabrication) on the shortened rod geometry. FGR calculations during the base irradiation provide a value of 1.48% for FRAPCON coupled with SCIANTIX, 2.02% for OFFBEAT coupled with SCIANTIX, and 2.47 for TRANSURANUS coupled with SCIANTIX. As for the ramp test, code calculations for the FGR provide values of 9.9% for FRAPCON coupled with SCIANTIX, 10.1% for OFFBEAT coupled with SCIANTIX, and 11.7% for TRANSURANUS coupled with SCIANTIX.

3.8. *HATAC C2*

3.8.1. *Experiment description*

The HATAC project belongs to the IAEA FUMEX-II benchmark [69] and consisted of two tests (fuel rod C1 and fuel rod C2) aimed at analysing FGR mechanisms in UO_2 at medium burnup, and during power cycling operations. Due to the better availability and quality of the experimental data and the burnup range, we consider the rod C2. The HATAC C2 fuel rod was base-irradiated in the Fessenheim-1 Nuclear

Table 4
Design data of the HATAC C2 fuel rod [74].

Parameter	HATAC C2
Fuel rod	
Initial diametrical gap size (mm)	0.191
Fuel stack height (m)	3.6594
Total gap volume (cm^3)	15.2
Filling gas	He
Initial gas pressure (bar)	34.5
Plenum height (cm)	15.77
Cladding	
Alloy	SRA Zircaloy
Outer diameter (cm)	0.9524
Inner diameter (cm)	0.8384
Fuel pellets	
Fuel	UO_2
^{235}U enrichment (%)	3.138
Pellet outer diameter (cm)	0.8193
Pellet height (cm)	1.401
Dishing number per pellet	2
Dish hemispheric radius (cm)	1.473
Dish depth (cm)	0.0305
Relative density (% TD)	93.984
Volume density (g cm^{-3})	10.301
Average grain size (μm)	7.05 to 7.99
Open porosity (%)	0.1
Spring	
Material	Steel AISI 302
Wire diameter (cm)	0.1705
Spire diameter (cm)	0.815
Number of spires	45

Power Plants (NPPs) up to an average burnup of 45.79 MWd kgU^{-1} (four irradiation cycles). Then, the fuel rod segment was extracted from the mother rod and re-irradiated in the SILOE reactor. The re-irradiation included a sequence of short power transients at LHR between 18-20 and 28-29 kW m^{-1}. Power holding lasted approximately three hours, at a ramp rate of about 5 kW m^{-1} min^{-1}. The rod segment was equipped with a gas sweeping device to measure amount and kinetics of stable and radioactive gases released during transients. A more detailed description of the irradiation conditions can be found in [23,74]. The specifications of the HATAC C2 mother rod are summarised in Table 4.

3.8.2. Simulation results

The HATAC C2 fuel rod is simulated with TRANSURANUS, OFFBEAT, and FRAPCON, coupled with SCIANTIX 2.0. The FGR calculated with the three codes is shown in Fig. 9a, with the experimental measurement of about 0.4%.

In line with usual fuel rod simulations, only the refabricated section is simulated during the power cycling test. The refabricated height of the active fuel was 282.4 mm, with an upper plenum of about 68.4 mm. Moreover, the pressure in the refabricated fuel rod circuit operated between 0 and 4 bars, but since no detailed pressure readings were provided, the rod internal pressure was set to 1 bar. The FGR calculated with TRANSURANUS, OFFBEAT, and FRAPCON is represented in Fig. 9b.

4. Discussion

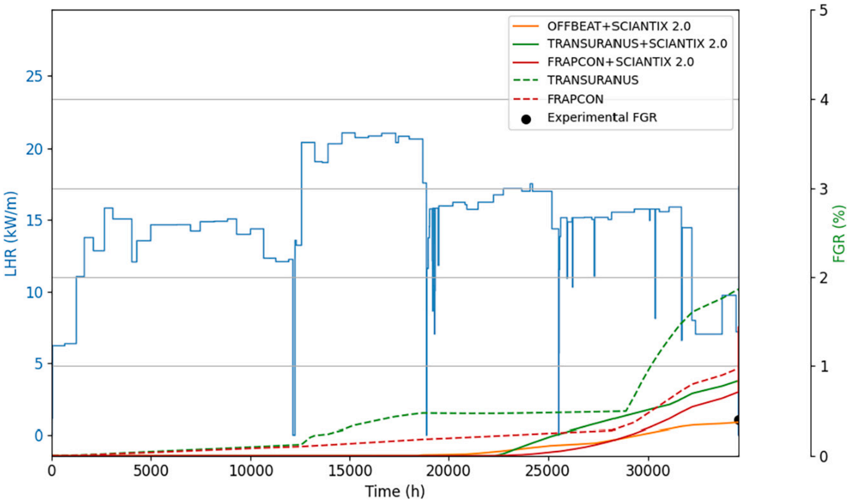
The previous section illustrated the performance of FRAPCON, TRANSURANUS and OFFBEAT coupled with SCIANTIX (version 2.0) when applied to the simulation of LWR fuel rods. The analysis also includes results from standalone FRAPCON and TRANSURANUS codes, using their default FGB formulation.

The end-of-life FGR values illustrated in Fig. 5a for the base irradiation of the AN3, Fig. 8a for the REGATE base irradiation, and Fig. 9a for the HATAC C2 base irradiation, demonstrate a qualitative agreement with the experimental data. The results at the end of the irradiations also align with the empirical description available in TRANSURANUS and FRAPCON. The comparison can be considered satisfactory and acceptable in light of the typical uncertainties in the calculated FGR during LWR base-irradiation condition, i.e., more than a factor 2 of deviation with respect to the experimental observations. As for the performance of SCIANTIX 2.0 coupled with TRANSURANUS, FRAPCON and OFFBEAT, applied in transient conditions, the results illustrated in the previous sections show the FGR kinetics during rapid power transients (i.e., the AN3 bump test in Fig. 5b, the single REGATE ramp test in Fig. 8b, and the cycled HATAC C2 ramp test in Fig. 9b). Among the cases analysed in detail, the agreement is satisfactory for the REGATE and HATAC C2 cases. However, in the Risø-3 AN3 case, the gas released during the bump test is underestimated. Such under-prediction is partially ascribable to measurement techniques since the FGR was retrieved from the rod internal pressure. A better description of the burst release due to micro-cracking, considering fragmentation contribution, gap and fuel cracks reopening during power reduction, is of interest for future developments. Some degree of uncertainty is ascribable to the inherent modelling choices pertaining to the integral codes. For instance, the macroscopic cracking of the fuel is considered in slightly different ways in the three codes. The OFFBEAT code includes the work of Barani et al. [75] with an increasing number of fuel cracks. The TRANSURANUS default option considers a fixed number of cracks, while FRAPCON includes the description from Oguma et al. [76]. A detailed comparison of the different FPC settings may be of interest for future works. In light of the intrinsic modelling and experimental uncertainties, SCIANTIX 2.0 predictions can be considered acceptable, paving the way for possible model improvement.

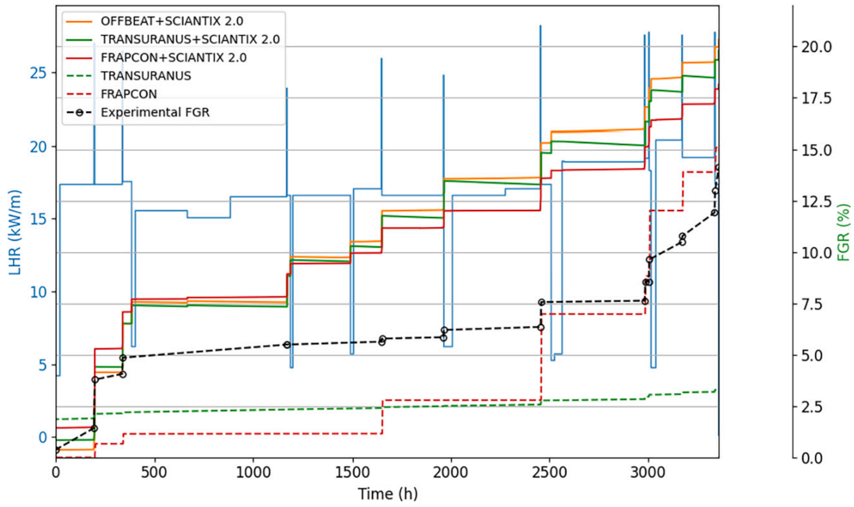
Such discussion also holds for the CONTACT1 irradiation experiment, where online measurements of the FGR are available, and for which TRANSURANUS and OFFBEAT coupled with SCIANTIX 2.0 predict a FGR in qualitative agreement with the data (Fig. 7a). The CONTACT1 irradiation experiment had indeed a peculiar setup, namely, a short UO_2 fuel rodlet irradiated at relatively high LHR (about 40 kW m^{-1}) during several short cycles, at imposed rod internal pressure. As for the capability of SCIANTIX 2.0 to track radioactive fission gases, Fig. 7b demonstrates the transfer of a meso-scale description up to the integral scale of the fuel rod. The release kinetics for short-lived ^{133}Xe agrees with the experimental data, especially when compared against the empirical approach [1], which essentially follows the linear power.

Fig. 10 collects the FGR deviation factor obtained from the FPCs coupled with SCIANTIX 2.0 as a function of calculated FGR values. Fig. 10 also includes the deviation factor curve obtained by Pastore and coauthors [39] after the uncertainty and sensitivity analysis on typical FGB uncertainty parameters. Numerical values are listed in Table 5, together with calculated deviation factors. From Fig. 10, it emerges how FGR calculated with FPCs coupled with SCIANTIX 2.0 are enclosed within a reasonable accuracy range. This is valid both at large FGR regimes (above 5 - 10%), namely, where the typical diffusion-based mechanisms are well-established, and where burst release mechanisms trigger significant release of fission gases, but also in the low FGR regime, typical of LWR base-irradiation conditions. Such low FGR region is notably more susceptible to uncertainties associated with gas release, e.g., driven by athermal mechanisms [77]. Hence, significant deviation factors typically occur.

Summarising, from the performance of the codes considered in this work, it emerges how the physics-based approach employed in SCIANTIX 2.0 provides a compelling description, alternative to conventional semi-empirical approaches. As already mentioned, by using SCIANTIX as FGB module, FPCs automatically inherit new modelling features (e.g., physics-based description, burst release model, radioactive gas release), and they can be used in stationary and transient conditions. Future model improvement can be transferred with a minor effort to the FPCs, and developments of interest for fuel performance analysis include the description of the HBS connected to the fuel fragmentation [17,24,25,70], the description of the athermal fission gas release due to grain-boundary open porosity [77], the modelling of doped fuels by



(a) HATAC C2 - Base irradiation: Fission gas release. The black dot represents the fission gas release measured at the end of the base irradiation. The solid lines are the calculations of the considered FPCs coupled with SCIANTIX 2.0, namely, OFFBEAT (orange line), TRANSURANUS (green line), and FRAPCON (red line). The dotted lines are default calculations of TRANSURANUS (green) and FRAPCON (red). The blue y-axis on the left reports the LHR imposed in the irradiation history.



(b) HATAC C2 - Power cycling: Fission gas release. The grey symbols represent the fission gas release calculated during the experiment: The black circles represent online measurement of FGR, connected with dotted lines to enhance readability. The solid lines are the calculations of the considered FPCs coupled with SCIANTIX 2.0, namely, OFFBEAT (orange line), TRANSURANUS (green line), and FRAPCON (red line). The dotted lines are default calculations of TRANSURANUS (green) and FRAPCON (red). The blue y-axis on the left reports the LHR imposed in the irradiation history.

Fig. 9. Results of the HATAC C2 fuel rod simulation. Calculations are performed with TRANSURANUS, FRAPCON, and OFFBEAT coupled with SCIANTIX 2.0 and with the default versions of TRANSURANUS and FRAPCON.

adding new fuel materials directly in SCIANTIX [29], and the application of machine learning techniques in FPCs [78]. Lastly, as for the execution time of SCIANTIX coupled with integral codes, we report an increase in the simulation time of a factor of two or three, depending on the simulated case. Such a time increase may be somehow less critical when fast-running codes. On the other hand, more efficient CPU management is of great interest to further reduce the computational time.

5. Conclusions

This work outlines the comprehensive integral validation of the meso-scale code SCIANTIX, coupled to the FPCs FRAPCON, TRANSURANUS, and OFFBEAT. The codes are applied in both base-irradiation and transient conditions, focusing on LWR fuel rod analysis. Within the integral codes, SCIANTIX (version 2.0) provides fast and accurate calculations of the fission gas released. Considering various inter-related gas and bubble behavioural models, the stable intra/inter-granular FGB formulation yields satisfactory agreement with experimental data during base-irradiation and transient conditions. The agreement is generally good, considering the typical uncertainties and complexities related to model parameters and experimental measurements. Nevertheless, the overall performance of SCIANTIX 2.0 in these conditions remains acceptable, and most importantly, it suggests its potential application in industrial FPCs. The automatic inheritance of meso-scale capabilities appears to be a strong and versatile feature that may shorten the time required in future model developments, from lower-length to engineering scale, including information from separate-effect experiments (e.g., conducted on single fuel grains) and atomistic-scale simulations. In summary, this work not only provides a comprehensive, integral validation of the SCIANTIX 2.0 meso-scale code when applied to LWR fuel rod con-

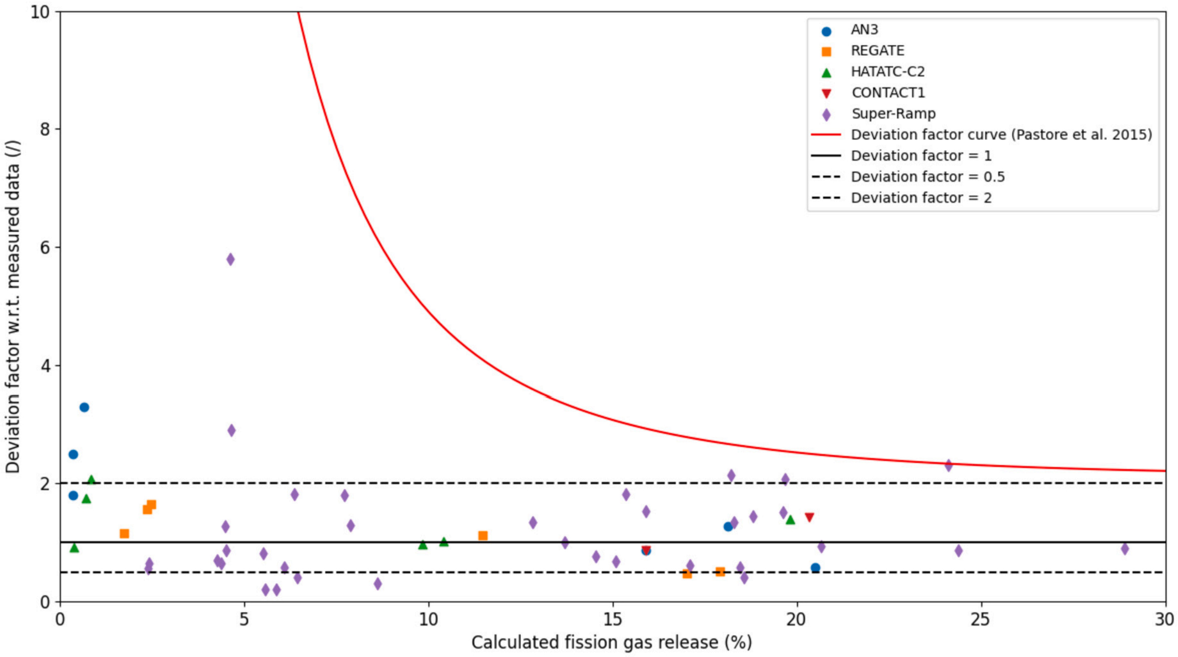


Fig. 10. Deviation factors as a function of FGR values computed by FPCs coupled with SCIANTIX 2.0. The figure includes the sensitivity analysis obtained by Pastore and co-authors [39] as a solid red line. The dots represent end-of-life FGR calculations obtained for the considered cases.

Table 5
Summary of the end-of-life calculated FGR (%). All the calculations are referred to FPCs coupled with SCIANTIX 2.0. The deviation factor (calculated/measured) is enclosed within the brackets.

	Measured	TRANSURANUS	FRAPCON	OFFBEAT
AN3 (base)	0.2	0.66 (3.3)	0.35 (2.5)	0.36 (1.8)
AN3 (ramp)	35.5	20.51 (0.58)	17.02 (0.48)	17.92 (0.504)
REGATE (base)	1.5	2.47 (1.65)	1.73 (1.15)	2.36 (1.57)
REGATE (ramp)	10.2	11.48 (1.12)	9.84 (0.96)	10.41 (1.02)
HATAC C2 (base)	0.4	0.83 (2.07)	0.70 (1.75)	0.37 (0.92)
HATAC C2 (ramp)	14.14	19.81 (1.40)	18.13 (1.28)	20.32 (1.43)
CONTACT1	18.5	15.9 (0.86)	-	14.55 (0.77)
Super-Ramp				
PK1-1	8.5	18.20 (2.14)	-	15.35 (1.81)
PK1-2	13.6	18.31 (1.35)	-	13.71 (1.01)
PK1-3	22.1	20.66 (0.93)	-	15.10 (0.68)
PK1-4	13.0	18.81 (1.45)	-	19.64 (1.51)
PK2-1	28.0	24.38 (0.87)	-	17.11 (0.61)
PK2-2	32.1	28.90 (0.90)	-	18.45 (0.57)
PK2-3	44.9	30.33 (0.67)	-	18.58 (0.41)
PK2-4	9.5	19.68 (2.07)	-	12.83 (1.35)
PK2-S	10.4	24.12 (2.32)	-	15.91 (1.53)
PK4-1	10.8	-	-	6.10 (0.57)
PK4-2	16.2	-	-	6.44 (0.40)
PK4-3	29.0	-	-	8.63 (0.30)
PK4-S	29.0	-	-	8.63 (0.30)
PK6-2	28.4	5.88 (0.21)	-	5.57 (0.20)
PK6-3	3.5	6.37 (1.82)	-	4.48 (1.28)
PK6-S	6.7	5.51 (0.82)	-	4.37 (0.65)
PK3-2	6.1	7.89 (1.29)	-	4.26 (0.70)
PW3-3	4.3	7.73 (1.80)	-	2.39 (0.56)
BK7-3	1.6	-	-	4.64 (2.90)
BK7-4	0.8	-	-	4.63 (5.79)
BK7-5	5.2	-	-	4.52 (0.87)
BK7-6	7.0	-	-	4.75 (0.68)

ditions but also identifies the role of meso-scale codes as valuable tools for advancing and understanding fuel rod complex behaviour.

CRediT authorship contribution statement

G. Zullo: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Data curation, Conceptualization. **D. Pizzocri:** Writing – review & editing, Visualization, Validation, Supervision, Software, Methodology. **A. Scolaro:** Writing – review & editing, Supervision, Software, Methodology. **P. Van Uffelen:** Writing – review & editing, Validation, Supervision, Methodology. **F. Feria:** Writing – review & editing, Validation, Supervision. **L.E. Herranz:** Writing – review & editing, Validation, Supervision, Methodology. **L. Luzzi:** Writing – review & editing, Visualization, Validation, Supervision, Methodology, Funding acquisition, 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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