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A multi-fidelity multi-scale methodology to accelerate development of fuel performance codes

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ABSTRACT

Multi-scale methodologies have been developed and applied successfully in the frame of nuclear fuel performance analyses, but the complexity of the tools involved hinders their extensive application. Gaps in modelling capabilities of specific input/outputs in particular limits code-to-code communication. In this work, we propose a multi-fidelity methodology to tackle this issue. The application presented here concerns the inclusion of a meso-scale module describing fission gas behaviour (SCIANTIX) in a fuel performance code (FRAPCON). A critical input parameter of the meso-scale module, the local hydro-static stress in the fuel, is not predicted by such fuel performance code, hence limiting this coupling. This gap is filled by using a second fuel performance code (TRANSURANUS) to construct a virtual dataset of local hydro-static stress values, on which an artificial neural network is trained and included in the FRAPCON/SCIANTIX coupled suite. This multi-fidelity methodology is demonstrated by simulating the Risø AN3 irradiation experiment.

1. Introduction

The simulation of the nuclear fuel rod behaviour under irradiation is inherently a multi-scale task since it requires the description of phenomena occurring at microscopic time and length scales which impact the macroscopic performance of the fuel itself (Tonks et al., 2017; Van Uffelen et al., 2019; Capps et al., 2023). Among these phenomena, fission gas behaviour has been tackled by several authors at all scales. A development strategy that has been pursued in several simulation environments is the direct coupling of fuel performance codes (engineering-scale thermo-mechanical tools) with meso-scale point-like codes describing fission gas behaviour at the scale of a fuel grain (e.g., SFPR/MFPR-R (Veshchunov et al., 2013; Tarasov et al., 2023), BISON/SIFGRS&SIFGRSX (Pastore et al., 2015; Williamson et al., 2016), TRANSURANUS/FISPRO&MFPR-F&SCIANTIX (Pastore et al., 2013; Pizzocri et al., 2020; Zullo et al., 2023b,a, 2022a,b), ALCYONE/CARACAS (Jomard et al., 2014), GERMINAL/MARGARET (Lainet et al., 2019; Noirot, 2011), OFFBEAT/SCIANTIX (Scolaro et al., 2020). Such meso-scale codes can in turn be informed from lower-length scale calculations/ experiments and thus allow for direct online transfer of knowledge towards fuel performance codes. A more recent development trend is to conceive meso-scale codes describing fission gas behaviour for coupling with generic fuel performance codes (Zullo et al., 2023a). This development strategy has the advantage of easing the implementation and testing of new models within the meso-scale code, including their verification and separate effect validation. On the other hand, the coupling between the meso-scale code and the fuel performance code becomes a topic of its own, involving dedicated implementation efforts and numerical treatments such as time-step control or sub-time stepping strategies.

Among the development actions required to couple a meso-scale code with a fuel performance code effectively, it must be ensured that all the local values of physical variables required for the meso-scale code to perform its calculations are predicted by the fuel performance code (e.g., the local temperature field, the local fission rate density or specific power). If the fuel performance code considered in the coupling scheme does not have the predictive capabilities for such local variables, the overall meso-scale coupling approach is hindered. In this work, we investigate one of such coupling schemes, aimed at increasing the predictive capabilities of a legacy fuel performance code with respect to fission gas behaviour and targeting the extension of its

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[1] This work was conducted with access to both the TRANSURANUS and FRAPCON fuel performance codes, reflecting the broader context of institutions in the fuel performance community. The methodology developed in this work aims to facilitate the integration of meso-scale modules with fuel performance codes, making it more applicable. Moreover, the approach is not limited to modelling fission gas behaviour but can also be extended to other modules of fuel performance codes, such as burnup analysis, where a detailed understanding of local neutron flux is essential.

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validation database with irradiation experiments involving fission-gas-related figures of merit. On the fission gas behaviour side we consider SCIANTIX (Pizzocri et al., 2020; Zullo et al., 2023a), which requires as input the local temperature, fission rate density, and hydrostatic stress, while on the fuel performance side we consider FRAPCON (Geelhood et al., 2015; Geelhood and Luscher, 2015; Geelhood, 2016), for which the standard thermo-mechanical model of the fuel predicts local temperature and fission rate density, but not the local hydrostatic stress. The standard way around such limitations would be to either implement in FRAPCON, i.e., the legacy code, new modelling capabilities or to use a limited version of SCIANTIX, i.e., the meso-scale model. Both these strategies face several limitations, such as the formal requirements connected with updating licensed codes (see Autorite de surete nucleaire - ASN and Institut de radioprotection et de surete nucleaire - IRSN and IRSN (2017) as examples) or the need to re-evaluate the separate effect validation of meso-scale codes with limited inputs/parameters. As an alternative to these approaches, we propose a multi-fidelity methodology tailored on a specific irradiation experiment and involving another legacy code (i.e., TRANSURANUS) that is used in parallel to FRAPCON to provide that information required by the meso-scale code (i.e., the local hydrostatic stress in the fuel) that are not available in its standard model[1]. This application is made possible using machine learning techniques such as artificial neural networks to achieve competitive computational times. The methodology is outlined in Section 2, while Section 3 describes the application to the selected irradiation experiment (the widely analysed AN3 irradiation experiment (Chantoin et al., 1998; Barani et al., 2017; Wu et al., 2018; Scolaro et al., 2022) and to the specific figure of merit (hydrostatic stress). The results are collected and discussed in Section 4.

2. Methodology

To couple a meso-scale module describing fission gas behaviour with a fuel performance code, the values of several physical variables calculated[2] by the two coupled codes need to be exchanged, typically:

- From the fuel performance code to the fission gas behaviour module: local fuel temperature, local burnup, local fission rate, local hydrostatic stress in the fuel, …
- From the fission gas behaviour module to the fuel performance code: local swelling, local contribution to fission gas release, …

If one (or more) of the required physical variables are not calculated by either the fuel performance code or the fission gas behaviour module, is it still possible to construct an effective coupling scheme? This question has to be answered when targeting the inclusion of SCIANTIX in FRAPCON, since FRAPCON does not calculate the local hydrostatic stress in the fuel[3] which is a required input for SCIANTIX models. The fuel hydrostatic stress is accounted for in the estimation of the over-pressurization of grain-boundary bubbles, which determines their inflow of vacancies.

$$\frac{\mathrm{d}n_v}{\mathrm{d}t} \sim \left(p - \frac{2\gamma}{R} + \sigma_h\right) \tag{1}$$

where $\mathrm{d}n_v/\mathrm{d}t$ (vacancies m^{-3} s^{-1}) is the vacancies inflow in grain-boundary bubbles, p (Pa) is grain-boundary bubble pressure, $2\gamma/R$ (Pa) is the equilibrium pressure, with γ (N m^{-1}) being the surface tension and R (m) is the projected bubble radius, and σ_h (Pa) is the hydrostatic stress. With compressive (negative) hydrostatic stresses in the fuel, the inflow of vacancies is reduced, and therefore the growth of grain-boundary bubble is slower, which slows the gaseous swelling rate and postpones the onset of fission gas release. The interaction between fission gas behaviour and hydrostatic stress in the fuel goes also in the other way, since less fuel swelling translates in a milder pellet-cladding mechanical interaction, hence less contact pressure and less hydrostatic stress in the fuel. The impact in engineering scale simulations of considering the hydrostatic stress in Eq. (1) has been extensively demonstrated by Pastore et al. (2013) and subsequent studies, e.g., Pastore et al. (2015), Barani et al. (2017). To include such a mechanistic description of fission gas behaviour in the FRAPCON code, the methodology depicted in Fig. 1 is set in place. The RisøAN3 irradiation experiment is chosen to demonstrate the application. The process has two different phases: an offline training phase and a simulation phase. During the offline training phase, the irradiation experiment is simulated with TRANSURANUS (Lassmann, 1992), which has the capability to predict the hydrostatic stress in the fuel. These results are used to construct a virtual dataset based on which an artificial neural network is trained. The obtained neural network and SCIANTIX are coupled with FRAPCON. In the online phase, FRAPCON/SCIANTIX, complemented with the artificial neural network for hydrostatic stress, is used to simulate the irradiation experiment.[4] In this way, a multi-scale simulation is possible even if the codes involved lack part of the predictive capabilities required, with the gap covered by a multi-fidelity offline calculation embodied in the multi-scale tool via machine learning.

The obtained ANN depends on the TRANSURANUS calculations, i.e., the training dataset. The feedback mechanisms of fission gas behaviour on the stress field in the fuel depend on the state of the fuel-cladding gap. Two situations are identified:

- Open gap: The feedback is primarily thermal, affecting gap conductivity and gap size, which in turn influence the fuel temperature, material properties, and stress levels. Additionally, fission gas release increases the internal rod pressure, raising the compressive hydrostatic stress in the fuel. However, these effects are secondary to the direct influence of hydrostatic stress on constraining bubble growth, thereby reducing the fuel swelling rate.
- Closed gap: The feedback is predominantly mechanical. Fuel swelling contributes to the contact pressure between the fuel and the cladding, which acts as a compressive boundary condition. This directly increases the hydrostatic stress in the fuel, representing the main source of interdependency between the stress field and fission gas behaviour.

3. Application

The proposed methodology is applied to the RisøAN3 irradiation experiment (Chantoin et al., 1998), a ramp test conducted at the RisøDR3 water-cooled HP1 rig using a re-fabricated rod from a pressurized water reactor. The mother rod, CB8, was irradiated over four reactor cycles up to a burnup of 41 $\mathrm{GWd/t_{UO_2}}$ and re-fabricated to a

[2] Different coupling strategies can be conceived that imply different calculation strategies for such coupling variables. In this sense, the term "local" is to be intended with a specific meaning in each specific application, e.g., referring to the average value of a variable in a mesh cell (e.g., for finite volume tools like OFFBEAT/SCIANTIX (Scolaro et al., 2022)), or to the value of variable in a quadrature point (e.g., for finite elements tools like BISON/SIFGRS (Williamson et al., 2016)), and so on.

[3] FRAPCON assumes a "rigid pellet" model for the fuel, i.e., the FRACAS-I model (Geelhood et al., 2015) which neglects the stress-induced deformation of the fuel and in turn implies that no local stress is calculated in the fuel.

[4] While it is possible to feed FRAPCON with a uniform, radially-averaged, hydrostatic stress using a similar ANN, we opted to compute the complete radial profile of the hydrostatic due to the manageable computational effort of the ANN. It is worth noting that the default fission gas behaviour model in FRAPCON equates the hydrostatic stress in the fuel (S_{hyd}) to the gap pressure (P_{gap}). Alternative approaches include replacing this value with the sum of the gap pressure and contact pressure ($P_{\mathrm{gap}} + P_{\mathrm{c}}$) or using a linear scaling such as $S_{\mathrm{hyd}} = P_{\mathrm{gap}} + \frac{2}{3}P_{\mathrm{c}}$, as proposed in the work of Jernkvist (Jernkvist, 2019).

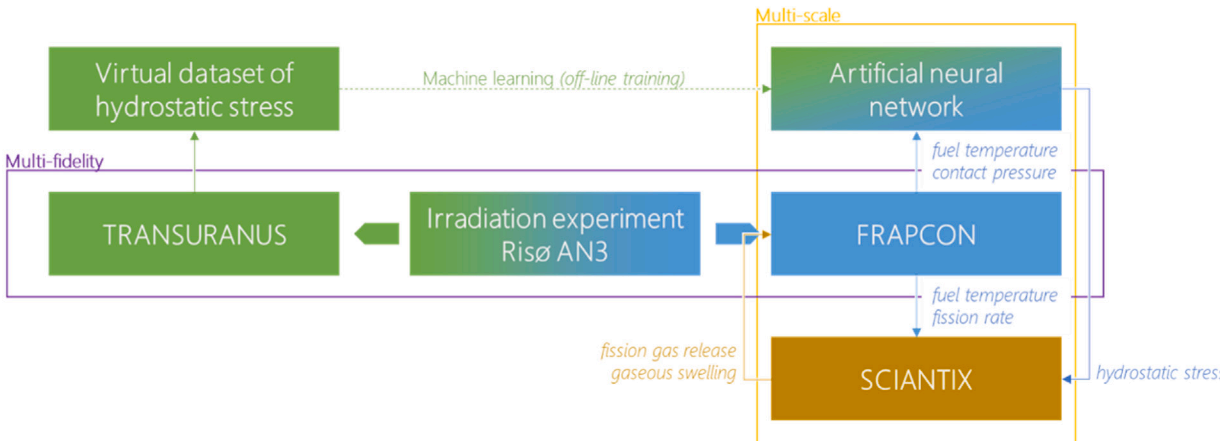

Fig. 1. Development scheme of the FRAPCON/SCIANTIX system using an artificial neural network as surrogate model.

Table 1
Validation range of the trained neural network.

Input parameters	Range
Fuel outer radius (mm)	(0, 4.6)
Burnup (MWd/kgU)	(0, 40)
Contact pressure (MPa)	(0, 42.1)
Gap pressure (MPa)	(1.2, 6.4)
Maximum fuel temperature (°C)	(20, 1968.7)
Minimum fuel temperature (°C)	(20, 493.5)

shorter length. The re-fabricated CB8-2R rod was instrumented with a fuel centre thermocouple and a pressure transducer[5] (Chantoin et al., 1998). The offline training phase of the proposed methodology is performed by simulating the base irradiation and the ramp test of the RisøAN3 irradiation experiment with TRANSURANUS. From this simulation results, the hydrostatic stress radial profile is extracted at each axial position[6] as a function of time, together with the time-evolution of the parameters used to predict it at each axial position, i.e., the normalized position along the fuel radius, the section average rod burnup, the contact pressure between fuel and cladding, the gap pressure, the fuel central temperature, and the fuel surface temperature. These six parameters physically drive thermal and mechanical stresses in the fuel during irradiation and are thus used as input parameters for the artificial neural network. The validation range of the trained artificial neural network is reported in Table 1.

The artificial neural network used in this application is a feedforward neural network with a single layer of ten neurons, six inputs (the parameters listed above), and one output (the local hydrostatic stress in the fuel). The training has been performed with the Levenberg–Marquardt algorithm (Levenberg, 1943; Marquardt, 1963, 2024) and the global mean square error as a cost function. Two data sets are used for the training: the first based on TRANSURANUS results with an open fuel-cladding gap, and the second with a closed gap. In total 70% of 10’000 datapoints are used to train the artificial neural network, with a random subset of 15% used for validation and another 15% for testing. As can be seen in Fig. 2, there is a qualitative agreement between the hydrostatic stress predicted by TRANSURANUS and by the artificial neural network paired with FRAPCON/SCIANTIX. The quantitative differences arise from the different input values calculated for the artificial neural networks by TRANSURANUS and FRAPCON respectively. In terms of the shape of the hydrostatic stress radial profile, there is a difference in the outer part of the fuel pellet. This is due to the difference between the variables computed by TRANSURANUS, used as a training dataset, and those computed by the FRAPCON/SCIANTIX as input for the artificial neural network. In the open gap dataset, the main difference arises from the values of the fuel temperature (both surface and central), which differ around 10%. In the closed gap dataset, the main difference is ascribed to the contact pressure, for which there is a factor of three between TRANSURANUS and FRAPCON/SCIANTIX. Moreover, the artificial neural network is constructed to conserve the symmetry boundary condition of the hydrostatic stress in the centre of the fuel pellet. It is worth noting that values of hydrostatic stress in the order of tens of megapascals surely impact the behaviour of fission gas bubbles, as observed experimentally by White and coauthors (White, 2004; White et al., 2006) and predicted by mechanistic models (Pastore et al., 2013; Barani et al., 2017; Pizzocri et al., 2020; Zullo et al., 2023a). The application of the proposed methodology to other irradiation experiments can be tackled in two different ways: the offline machine learning action can be performed by constructing an artificial neural network for each irradiation experiment considered, or a single neural network can be trained based on the combined datasets of several irradiation experiments.

4. Results

Fig. 3 reports the results in terms of fission gas release for the new FRAPCON/SCIANTIX coupling supported by an artificial neural network (FRAPCON/SCIANTIX-ANN). For comparison sake, we include results for FRAPCON standard fission gas model (Geelhood et al., 2015). The comparison is focused on the AN3 bump test, i.e., a re-irradiation of a re-fabricated rodlet in which the linear heat rate is progressively raised up to around 35 kW m^{-1} in roughly 30 h, and then hold for other 40 h. During the hold phase, the rodlet is subjected to two bumps in power. Along the bump test, a pressure transducer in the plenum records the internal rod pressure, correlated to fission gas release from the fuel. During these power bumps, a sudden increase in the pressure transducer records a sudden increase in temperature, which is attributed to a combination of gas being freed as pellet-cladding contact is relaxed and as gas being released from the fuel during the power transient as a result of grain-boundary micro-cracking (Barani et al., 2017). This second mechanism is physically connected with the levels of hydrostatic stress present in the fuel, also decreasing as the contact

[5] The measurement of the pressure transducer is converted from rod internal pressure to fission gas release via an ad hoc correlation originally developed ad Halden. In this work, we adopt a version of this correlation based on the findings of recent international benchmarks (NEA, 2024). The new correlation assumes a fission gas release 5% lower than the previous one during the all transient based on the understanding of a sensor malfunction at the beginning of the transient.

[6] TRANSURANUS is suited for this multi-fidelity role in the proposed methodology since it shares with FRAPCON a 1.5D geometric description of the fuel rod, thus not requiring a mapping of its hydrostatic stress results.

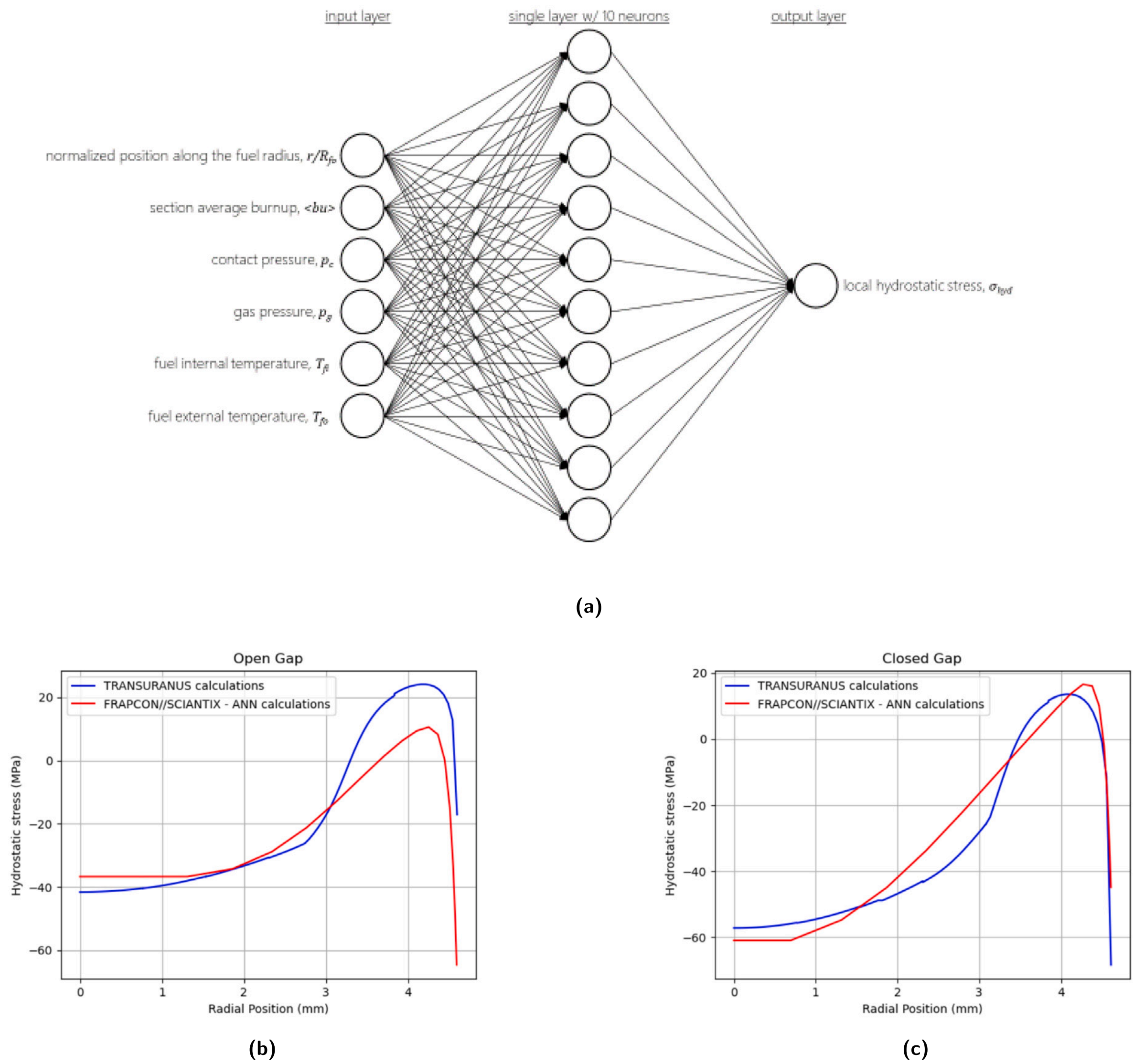

Fig. 2. (a) Structure of the artificial neural network used in this work and an example of its outputs in terms of local hydrostatic stress along radial position in open gap regime (b) and closed gap regime (c) as predicted by FRAPCON/SCIANTIX paired with the artificial neural network (ANN), compared with TRANSURANUS.

pressure between the fuel and the cladding decreases, and thus allowing for a growth of the grain-boundary bubble size during the transient.

The FRAPCON/SCIANTIX-ANN systems express quantitatively and qualitatively a good agreement with the experimental data, mainly since the coupling with SCIANTIX equips the code with a model for grain-boundary micro-cracking during temperature transients (Barani et al., 2017; Zullo et al., 2023a). This model is semi-empirical in its formulation, being tailored on separate effect experiments (e.g., Une and Kashibe (1990)), but still affects the size and number of grain-boundary bubbles and thus is linked to the hydrostatic stress via Eq. (1), and thus requires the integration of the artificial neural network described above. On the other side, the fission gas release model available in SCIANTIX is purely based on diffusion of gas atoms from inside the fuel grains to the grain boundaries, and fails at describing the transient behaviour observed in the experiment. The quantitative agreement with the final measurement point, obtained through puncturing of the fuel rodlet during post irradiation examination, confirms the improved descriptive capability brought about in FRAPCON by the coupling with SCIANTIX-ANN.

It is worth commenting that neither FRAPCON or FRAPCON/SCIANTIX-ANN (or any fuel performance code, to the knowledge of the authors) is able to describe the delayed detection of fission gas due to the re-opening of the fuel-cladding gap during the beginning of the bump transient. This limitation implies that a perfect agreement between the experimental data and the code predictions is not expected. Treatment of such dynamics of gas transport in the gap represents a key future development for the interpretation of the AN3 and similar irradiation experiments, and more in general for the description of fuel rods with breached claddings (Veshchunov and Shestak, 2009; Giaccardi et al., 2024).

As a last comment, even if the application of the proposed multi-fidelity multi-scale methodology improved FRAPCON predictive results of this specific irradiation experiments, further testing is targeted on the validation database of the code. This is the main reason for which it is out of the scope of this work to calibrate parameters in SCIANTIX-ANN, being the agreement with a single irradiation experiment a non-valuable target. Nevertheless, it is worth recalling that the application of such a methodology can allow the addition of new experimental cases to the validation dataset of a fuel performance code, and the demonstration case shown in this section should be seen as an exemplification of this process.

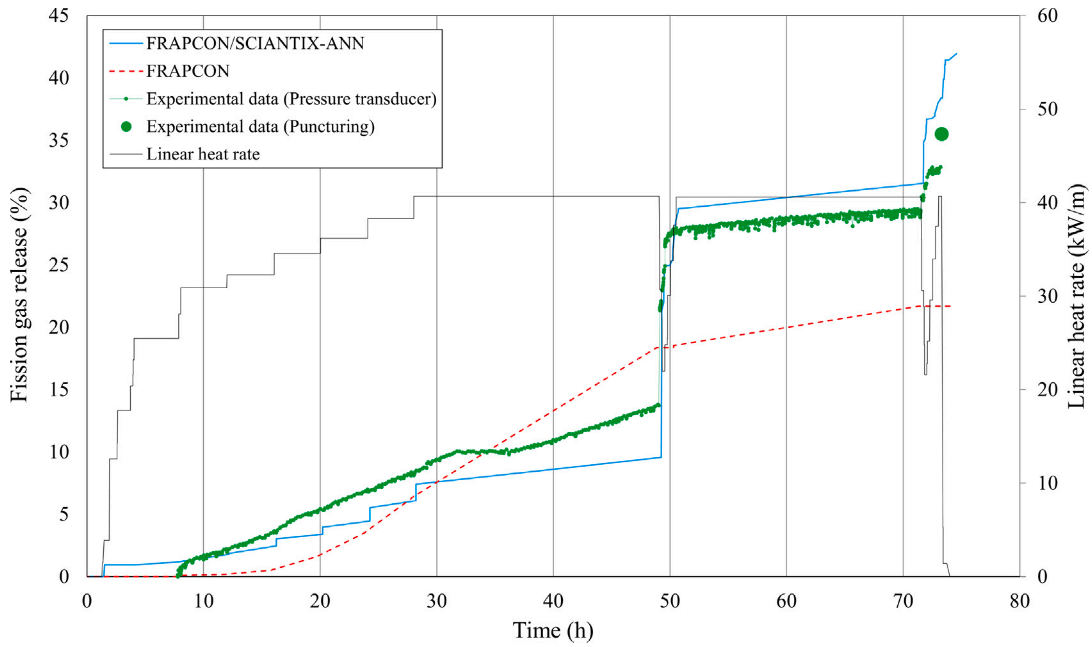

Fig. 3. Comparison of the code predictions (FRAPCON with standard model options and equipped with SCIANTIX-ANN for the description of fission gas behaviour) against the measured fission gas release along the RisøAN3 ramp test, both as measured via a pressure transducer during the irradiation (small green dots) and by puncturing during post irradiation examination (big green dot).

5. Conclusions

In this work, we proposed a methodology to allow for improving the predictive capabilities of reference fuel performance codes via a multi-fidelity multi-scale approach. The combination of a multi-fidelity tool enlarging the variables accounted for by the reference code is meant to allow for coupling the reference code itself with a multi-scale tool, thus equipping it with additional predictive capabilities. This methodology is demonstrated with the simulation of an irradiation experiment (RisøAN3) with FRAPCON, coupled with the meso-scale code SCIANTIX describing fission gas behaviour, and with the support of an artificial neural network (ANN) trained on offline TRANSURANUS calculations (i.e., the multi-fidelity tool) providing SCIANTIX the local values of hydrostatic stress which are not predicted in the standard FRAPCON code. The results of FRACON/SCIANTIX-ANN show both a qualitative and quantitative improvement with respect to the standard FRAPCON version when compared to experimental results, indicating that the proposed methodology is promising and should be extensively tested on the code validation dataset.

Given the promising results in the application case showcased in this work, we believe that a systematic use of the proposed methodology can represent a valuable support in extending the current predicting capabilities of fuel performance codes. One should also consider that the proposed methodology (1) leverages existing simulation tools, and (2) allows interpreting already available irradiation experiments, thus providing an efficient use of available resources in the research community. This aspect is relevant in view of the research initiatives promoting accelerated qualification of current codes for new fuel concepts.

CRediT authorship contribution statement

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

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: D. Pizzocri reports financial support was provided by Euratom Research and Training Programme. G. Petrosillo reports financial support was provided by EU Framework Programme for Research and Innovation Euratom. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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