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Towards simulations of fuel rod behaviour during severe accidents by coupling TRANSURANUS with SCIANTIX and MFPR-F

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ABSTRACT

Among the applications of the multiscale modelling approach in nuclear fuel rod performance, the coupling of integral thermo-mechanical fuel performance codes with lower-length *meso*-scale modules is of great interest. This strategy allows to overcome correlation-based approaches with mechanistic ones and test their application in accidental conditions. In this work, we explore the coupling between the TRANSURANUS fuel performance code and two *meso*-scale modules for fission gas/product behaviour: MFPR-F and SCIANTIX. These modules, coupled within TRANSURANUS, are assessed against the IFA-650.10 loss-of-coolant accident test to analyse their overall impact and highlight future developments toward mechanistic modelling of fission gas during accident scenarios.

1. Introduction

Thanks to the continuously increasing soft- and hardware developments, in combination with the growing availability of more and better (i.e., more detailed) experimental data (Cappia et al., 2022), high-fidelity simulations are becoming mainstream in many fields.

In the analysis of the nuclear fuel rod behaviour, attention has been given to the development of multi-scale and multi-physics simulation tools through coupling codes that operate at different length. Conventional fuel performance codes (FPCs), such as the TRANSURANUS code developed at Joint Research Center (JRC) in Karlsruhe (Lassmann, 1992; Magni et al., 2021) or the FRAPCON and FRAPTRAN codes developed at the Pacific Northwest National Laboratory (PNNL) (FRAPTRAN; FRAPCON-4.0: 2015), exploit several models and correlations to describe the complex behaviour of the whole fuel rod in an efficient way from the scale of the fuel and cladding microstructure to the engineering scale of the fuel rod.

As a complement to the conventional fuel rod analysis, detailed mechanistic *meso*-scale codes have started to be developed (Veshchunov et al., 2006; Pizzocri et al., 2020), to improve the empirical or semi-empirical correlation-based approaches employed in FPCs (Vitanza et al., 1979; Turnbull and Beyer, 2010; Turnbull, 2001; Rausch and Panisko, 1979). Being physically-informed the *meso*-scale codes should improve the overall FPC predictive capabilities and, most importantly, has the potential to increase the understanding of complex phenomena affecting the fuel behaviour, especially at high burnup regime, during design basis accidents or in storage conditions (Van Uffelen et al., 2019). In particular, attention has recently been paid to analysing the behaviour of high-burn-up fuel rods in order to extend the lifetime of existing nuclear reactors. It is also known that a non-negligible fission gas release can occur under such burn-up conditions. Approaches describing fission gas behaviour under operating conditions are often unable to capture the release of fission gas during accidental transients, hence mechanistic codes are currently candidates to extend fission gas models used in fuel performance codes (Rest et al., 2019).

In line with the current paradigm shift towards more mechanistic modelling of nuclear fuel rod behaviour (Van Uffelen and Pastore, 2020) and in particular the need for more detailed fission product simulations (Rest et al., 2019; Tonks et al., 2018), the present work outlines the coupling of the TRANSURANUS FPC with the mechanistic codes SCIANTIX (Pizzocri et al., 2020) and MFPR-F (Pavlov et al., 2018) that have been developed in parallel by different organisations, i.e., Politecnico of Milano (POLIMI) and Institut de Radioprotection et Sûreté Nucléaire (IRSN), respectively.

The mechanistic codes for fission gas and product behaviour SCIANTIX and MFPR-F are designed for coupling with integral thermo-

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mechanics FPCs. For example, the MFPR code (from which MFPR-F is derived) has been coupled with various tools in the SFPR and BERKUT modules (Veshchunov et al., 2015; Veshchunov et al., 2013), which in turn is used by the EUCLID/V1 FPC for fast reactors (Veprev et al., 2018). Recently, the SCIANTIX code has been coupled with the GERMINAL code (Lainet et al., 2019), the TRANSURANUS code (Zullo et al., 2022; Magni et al., 2022) for simulating FBR MOX fuel in the frame of the INSPYRE project (Magni et al., 2022). In the current work, we test the coupling of TRANSURANUS both with SCIANTIX and the MFPR-F code for simulating LOCA tests of pre-irradiated fuel in a commercial light water reactors (LWRs).

This work details the coupling of TRANSURANUS with MFPR-F and SCIANTIX and its application to a LOCA experiment (Halden IFA-650.10). The calculations of the version of TRANSURANUS coupled with both codes mentioned above remain almost unchanged in terms of the factors determining cladding ballooning and burst. However, the application of a mechanistic description to the behaviour of fission gas, which involves complex intra- and inter-granular phenomena, grasp a release of fission gas during the experimental transient that would otherwise not be captured. This constitutes an important milestone towards the application of mechanistic approaches for fission gas behaviour under accidental conditions in conventional fuel performance codes and is a prerequisite for an evaluation of fuel fragmentation, relocation and dispersal in a mechanistic way (Capps et al., 2020; Khvostov, 2020; Chung et al.; NEA, 2016).

Section 2 introduces the adopted simulations tools as well as their coupling. In Section 3 we apply the coupled code system to one LOCA experiment from the recent coordinated research project Fuel Modelling under accident conditions (FUMAC) of the IAEA (FUMAC-TECDOC; Veshchunov et al., 2018), and discuss the outcomes. In Section 4, we draw the conclusions of this work and outline perspectives for further development and application of the new high-fidelity tools. Lastly, in the Appendix we include a list of the code subroutines that have been modified for the code coupling and is therefore available for the user community of the TRANSURANUS fuel performance code.

2. The new coupled code system

2.1. The TRANSURANUS code

The simulation of a single fuel rod in this work relies on the TRANSURANUS code that was originally programmed in Fortran77 (Lassmann, 1992) and has been rewritten in modern Fortran for code coupling (García et al., 2020; García et al., 2021). The fuel rod performance code has been extended to deal with loss of coolant accident conditions (Van Uffelen et al., 2008), and has gradually benefitted from the inclusion of more mechanistic models for fission product behaviour (Pastore et al., 2013; Pastore, 2012). The latter provided the code with a mechanistic treatment of fission gas atoms at the (spherical) grain boundaries (contained in the FISPRO2 model of the code (Pastore et al., 2013; Pastore, 2012)), in addition to the standard model for the fission gas behaviour based on the conventional saturation concentration of gases at grain boundaries (White and Tucker, 1983; Forsberg and Massih, 1985; Forsberg and Massih, 1985) (contained in the FISPRO subroutines of the code (Lassmann et al., 2014). The mechanistic treatment (Pastore et al., 2013; Pastore, 2012) takes into consideration bubble growth and subsequent interconnection to form tunnel-like networks for release of fission gas to the free volume in the fuel rod, preserving the spherical geometry of the fuel grain (White, 2004). In parallel to these developments for the TRANSURANUS code, independent tools for a more detailed and comprehensive description of the fission product behaviour were developed by partner organisations. They are briefly outlined in the next two sections, along with a more detailed description of the interface applied for their coupling with the TRANSURANUS code that eventually allows to simulate the base irradiation of a nuclear fuel rod in a commercial nuclear power plant (NPP), followed by a test irradiation in an experimental device in a single run. These independent tools enable TRANSURANUS users to benefit from the capabilities offered by each code and their continuous developments.

The TRANSURANUS fuel performance code approximates the pin behaviour with an axisymmetric, axially stacked, one-dimensional radial representation (often referred to as 1.5D) (Magni et al., 2021). The fuel pin is therefore discretized in axial slices, or sections, and in radial coarse zones for the evaluation of the material properties. The coarse zones are in turn divided into finer zones to perform the numerical integrations needed for the thermo-mechanical analysis. Right from its inception (Lassmann, 1992), the TRANSURANUS code was carefully designed to reflect the structure of the problem, which is defined by:

- The analysis of the fuel pin behaviour at different times.
- The analysis of the different sections or slices at a specific time.
- The loop structure to obtain solutions of the various nonlinear problems in each section or slice.
- Driver programs for the various options (e.g., calling different options for fuel creep or thermal conductivity correlations depending on the material under consideration).

Consequently, the whole code is designed in levels, the three most important of which are shown in Fig. 1.

The uppermost level deals with the time-loop of the complete fuel pin, meaning that the thermal–mechanical fuel pin behaviour is calculated in each time step of the loop. The second level of the code deals with the loop over all the axial sections or slices of the fuel pin, whereas the third level deals with the solution of all equations in each slice or section.

The physical phenomena governing the behaviour of the nuclear fuel pin under irradiation are thus included in the third level of the overall thermo-mechanical analysis and encompass a wide set of interrelated processes driven by the local temperature, fission rate density, and applied stress. In the third level of the code, the specific call is thus also made to the fission product behaviour model (FISPRO), as illustrated in Fig. 2.

For the application of different fission gas behaviour models, the TRANSURANUS code structure thus lends itself perfectly for coupling with an external model. The coupling with the MFPR-F code of IRSN or SCIANTIX of POLIMI serve as good examples.

2.2. The MFPR-F code and its plugin for TRANSURANUS

The MFPR-F code of IRSN is derived from the MFPR code developed by Veshchunov and coworkers (Veshchunov et al., 2006). The code is programmed in modern Fortran, and currently for the coupling with TRANSURANUS it describes the behaviour of fission products, fuel thermochemistry as well as the formation and behaviour of point (vacancies and interstitials) and extended (interstitial dislocation loops and vacancy clusters) defects at each node of the fuel mesh. The validation database of the MFPR-F code (Veshchunov et al., 2006; Veshchunov et al., 2007; Veshchunov, 2000; Veshchunov and Shestak, 2008) contains separate-effects tests for validation of the individual models, as well as integral tests for LOCA (Pontillon, et al., 2004) and severe accidents (Ducros et al., 2013).

For the sake of the coupling with TRANSURANUS, a particular application program interface (API) was developed for use of MFPR-F as alternative to the recommended TRANSURANUS standard model (Lassmann et al., 2014), the TRANSURANUS mechanistic model (Pastore et al., 2013; Pastore, 2012), or the SCIANTIX code (Pizzocri et al., 2020), as it is sketched in Fig. 2.

The API permits TRANSURANUS to interface with MFPR-F for initialization, data transfer and to run the MFPR-F driver, without directly accessing MFPR-F internal routines. In doing so, a strict separation between the codes is preserved, thus avoiding any overlapping

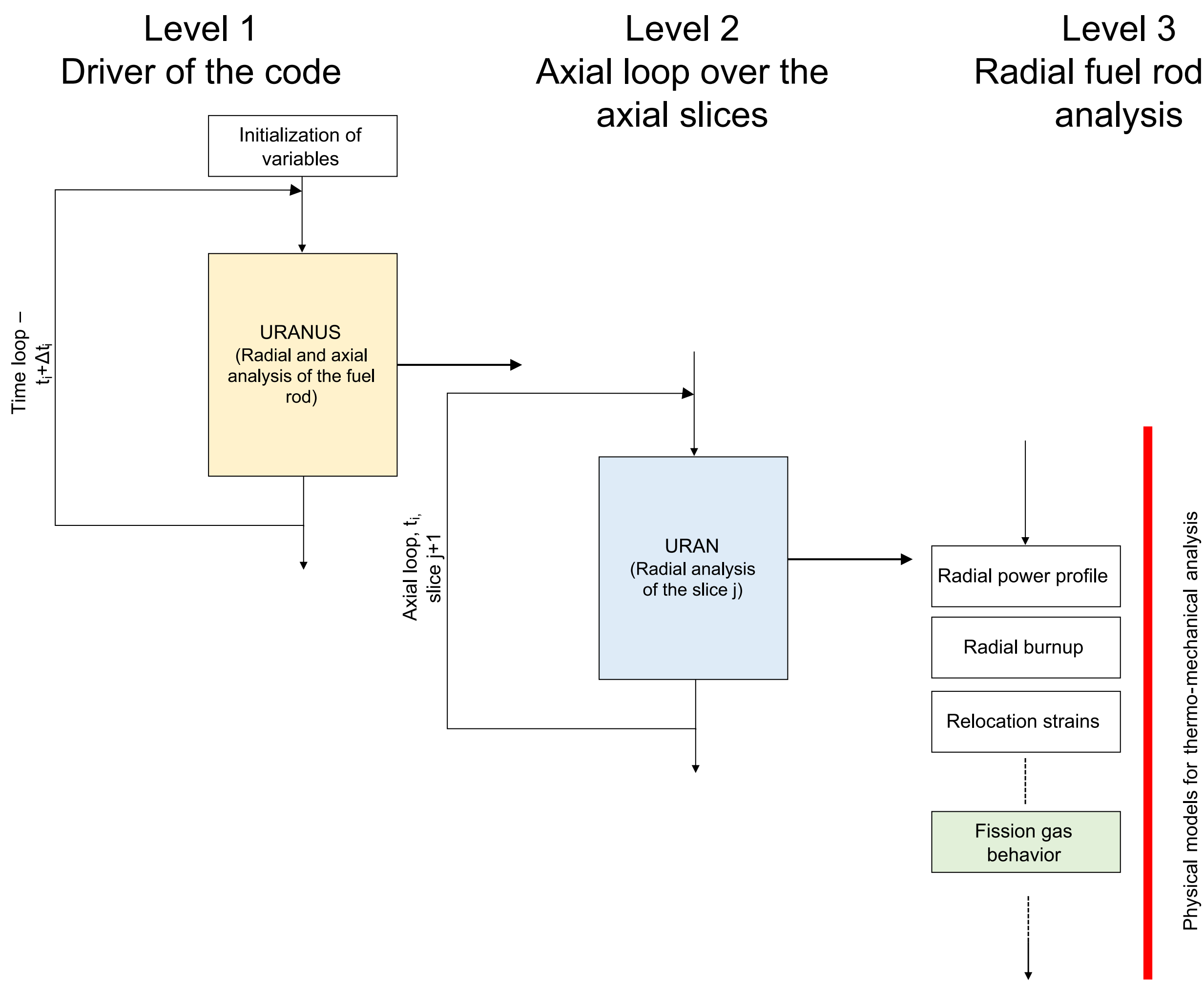

Fig. 1. Schematic flow chart and level structure of the TRANSURANUS code, and relevant sections modified for the modified fission gas behaviour modelling by means of code coupling (Pavlov et al., 2018).

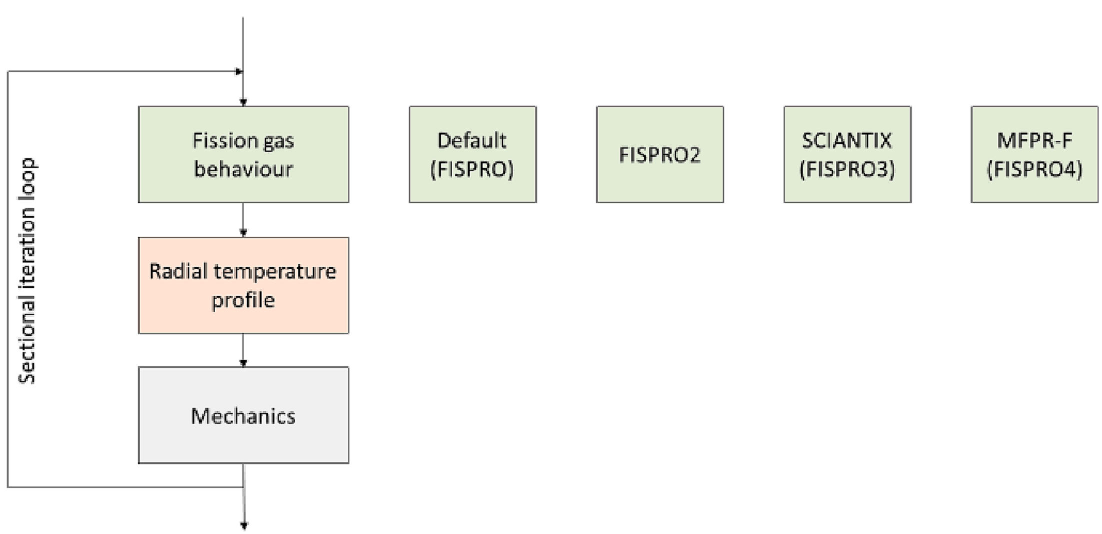

Fig. 2. Schematic flow chart of the level 3 in TRANSURANUS, driving the analysis of the fuel rod behaviour in a section or slice. The part of the flow chart shows the call to the *meso*-scale codes SCIANTIX and MFPR-F.

between them, which might alter future developments. To complement the API, a Fortran module was defined that declares common variables and acts as a buffer to transfer data, such as temperature and FP content, from TRANSURANUS variables to MFPR-F variables and vice versa.

Following the first coupling of the TRANSURANUS code with the MFPR-F code (Pavlov et al., 2018), the restart capability has been implemented. This is an essential feature that allows the coupled code system to handle the re-fabrication of a nuclear fuel rod segment in an experimental facility after base irradiation of the fuel rod in a commercial nuclear power plant. In particular, the restart capability requires storing MFPR-F internal variables in binary files and retrieving data from these files in the event of a restart calculation. A routine dedicated to these tasks was therefore created. It is based on an existing MFPR-F routine that performs the same tasks in the context of a stand-alone MFPR-F calculation.

2.3. The SCIANTIX code and its plugin for TRANSURANUS

SCIANTIX is a 0-D open-source computer code designed to simulate the fission gas behaviour in nuclear fuels (e.g., UO_2 or MOX), at the scale of the fuel grains (Pizzocri et al., 2020). The code can operate both as a stand-alone computer program and coupled to integral thermo-mechanical FPCs, if a suitable code interface is provided. SCIANTIX has been coupled with TRANSURANUS (Zullo et al., 2022; Van Uffelen, 2020), GERMINAL (Magni et al., 2022) and OFFBEAT (Scolaro et al., 2022).

The SCIANTIX validation database includes both separate-effect and integral irradiation experiments. In its standalone version, SCIANTIX physics-based models for inert gas behaviour have been validated against separate-effect experiments for intragranular and intergranular gaseous swelling (Pizzocri et al., 2020; White, 2004); (Baker, 1977), helium release and release rate experimental data (Cognini et al., 2021; Giorgi et al., 2022), and radioactive gas release experimental data (Zullo et al., 2022). Coupled with TRANSURANUS, SCIANTIX has been assessed against measurements of FGR, radioactive release, and radioactive release rate from UO_2 in stationary and transient conditions (Zullo et al., 2022; Faure-Geors et al., 1990; Bruet et al., 1980; Charles et al., 1983). Besides, the consistency of the numerical algorithms available in SCIANTIX (e.g., spectral diffusion algorithms for intragranular gas behaviour) is verified with state-of-the-art numerical techniques (Zullo et al., 2022; Oberkampf et al., 2002).

Concerning the coupling with TRANSURANUS, a specific API has been developed (Magni et al., 2022; Scolaro et al., 2022; Zullo et al., 2022; Van Uffelen, 2020). This API exploits Fortran and C++ standard intrinsic modules widely adopted scientific computation (Chapman, 2017), to ensure the interoperability between TRANSURANUS (Fortran) and SCIANTIX (C++). To minimize the effect on the existing structure of the TRANSURANUS code, and in line with the strategy adopted for the coupling with MFPR-F outlined above, TRANSURANUS interacts with SCIANTIX for initialization, data transfer and code execution, without directly accessing SCIANTIX internal routines, to avoid code overlaps that could interfere with future developments. Moreover, a second Fortran module was defined to declare variables common to TRANSURANUS and SCIANTIX, such as irradiation history variables (i.e., local temperature, fission rate density, hydrostatic stress, local burnup, and time step). Lastly, the SCIANTIX coupling is compatible with the TRANSURANUS restart option (Zullo et al., 2022), because all common variables are stored in binary files along with TRANSURANUS global variables.

3. Simulation of IFA-650.10 LOCA test with the new coupled code systems

In this section, the Halden IFA-650.10 LOCA experiment is described. Afterwards, results of the simulations performed with the TRANSURANUS code, coupled with SCIANTIX and MFPR-F, are presented. The IFA-650.10, from the international benchmark FUMAC organised by the IAEA, has been selected as representative benchmark case. It represents a case that can be readily simulated with the current versions (and all the implemented features) of both SCIANTIX and MFPR-F, coupled with TRANSURANUS, without the need to consider complicating factors related to fuel relocation (such as in IFA-650.9). The case is thus a reasonable starting point to add functionalities to simulate cases where FG behaviour is manifestly appreciable, e.g., IFA 650.9/12/13/14 (Khvostov, 2022).

3.1. Overview of the test

The Halden IFA-650.10 test belongs to the series of tests conducted on commercial irradiated fuel from 2005 to 2017, in pressurized flask connected to a water loop. The test that is considered in this work involved a rod segment with UO_2 fuel supplied by EDF/FRAMATOME (Pastore et al., 2021; FUMAC-TECDOC; Lavoil, 2010). The segment was cut from a standard rod which was pre-irradiated during five cycles in the French PWR Gravelines 5 (900 MWe) up to an average burnup of 61 MWd/kgU. Then, the segment was refabricated and filled with a gas mixture of 95% Ar and 5% He at 4 MPa, to represent the low-conductivity fission gases during a hypothetical LOCA. Manufacturing characteristics of the IFA-650.10 refabricated fuel rod used during the test are detailed in Table 1.

The experimental setup in the Halden reactor ensured that most of the energy for heating came from a low level of fission power in the fuel rod, simulating the decay heat. To reproduce the energy from the neighbouring rods, electrical heaters were installed surrounding the rod and acting as a flow path splitter.

The measurement tools included several thermocouples, cladding extensometer, and pressure transducer to detect fuel, cladding and coolant conditions (e.g., pressure and temperature).

In summary, the LOCA transient was executed according to the following procedure:

Initially, forced circulation was maintained through the pressure flask. Prior to blow-down, the pressure flask was isolated from the rest of the loop where circulation was maintained. The fuel rod was cooled by natural circulation in the pressure flask. The LOCA began when the valves were opened, starting the blow-down. The blow-down tank contained 15–20 L of water. The test was terminated by a reactor scream, the water was gradually cooled down without reflood and the steam from the flask was condensed. At the end of the blow-down, the pressure in the system was about 2–3 bar due to non-condensable gases.

The LOCA test was performed at a rod power of about 14 kW/m. The average cladding temperature increased from about 187 °C to a peak temperature of the cladding 850 °C, with an initial rate of 4–5 °C/s which decreased to 1 °C/s at the cladding burst. The burst was detected 249 s after the start of the blow-down, at about 755 °C and 7 MPa, and verified by the gamma scanning performed at Halden. After the burst, the rod pressure dropped instantaneously. In addition, fuel relocation was not observed during the test, as confirmed by gamma scan and post-irradiation examination (PIE).

417 s after the blow-down initiation, the experiment was terminated by switching off the electrical heating and scramming the reactor which caused the fission heat generation in the fuel rod to cease. The test rods were cooled down relatively slowly with the reactor to avoid disturbances, e.g., vibrations, which might possibly cause an unintentional

Table 1
Details of the IFA-650.10 refabricated rodlet (Veshchunov et al., 2018).

Fuel density (%TD)	95.32
Active fuel stack length (mm)	440
Initial enrichment (wt%U^{235})	4.49
Pellet outer diameter (mm)	8.21
Cladding outer diameter (mm)	9.50
Cladding thickness (mm)	0.57
Cladding diametral gap (μm)	150
Rod inner free volume (cm^3)	17
Cladding oxide thickness, irradiated (μm)	20–30
Cladding hydrogen content, irradiated (ppm)	150–220
Initial rod inner pressure (bar)	40
Rod filling gas	Ar (95%) + He (5%)

fuel relocation.

3.2. TRANSURANUS simulation setting

The rod linear heat rate (LHR) history was available through the FUMAC project and digitized to serve as TRANSURANUS input (FUMAC-TECDOC). Due to the number of involved participants (16 organizations) and to standardise different FPCs, thermal hydraulic boundary conditions (coolant temperature and clad-to-coolant heat transfer coefficient) were computed with the SOCRAT code, e.g., accounting for the electrical heater installed in the experiment (FUMAC-TECDOC; Kiselev, 2016).

In line with the simulations published in the FUMAC framework, the base irradiation (Fig. 3) was simulated on the refabricated rod geometry. The initial conditions for the transient simulation (Fig. 4) of the fuel segment are calculated by simulating the in-pile base irradiation. Both base and transient simulations are set according to the experimental specifications (e.g., Table 1) or the code manual recommended values (Lassmann et al., 2014). The refabrication stage is considered through the TRANSURANUS restart option, in which the initial moles of the new gas mixture of helium and argon are adapted to match the measured rod internal pressure at the start of the LOCA test.

3.3. Results

Fig. 5 shows the evolution of the fuel rod inner pressure during the blowdown phase of the IFA-650.10 test, as calculated by TRANSURANUS in its standalone version (blue line) and coupled with SCIANTIX (black line) and MFPR-F (red line), along with the experimental measurements (i.e., pressure transducer data, in green dots).

The calculations of the three versions of TRANSURANUS reproduce qualitatively the same behaviour for the fuel rod inner pressure. In particular, the codes follow the experimental behaviour with good accuracy until 100 s. After that, the inner pressure is always underestimated. This behaviour was justified within the FUMAC project as associated with the calculated cladding outward deformation (ballooning) and the overestimation in rod inner volume. This observation is also coherent with Fig. 6, showing the calculated cladding outer radius at the end of the simulation compared to the available PIE data.

The gap pressure is dependent on the gap volume and to the amount of gas it contains. These quantities are affected, in particular, by fuel swelling and FGR which occurred during the base irradiation. Hence, in Fig. 5, the differences that are visible, prior to burst, are a consequence of different results obtained during the base irradiation (e.g., cladding outer radius), combined with the use of the restart option to reproduce the refabrication stage.

Namely, the refabrication stage involves only the change in the gas composition and disregard the cladding deformation obtained during the base irradiation. By using TRANSURANUS coupled with SCIANTIX, the fission gas release at the end of the base irradiation is larger than the one obtained with the standalone version of TRANSURANUS, that is greater than the one obtained with TRANSURANUS coupled with MFPR-F. The amount of gas released affects the cladding expansion and the volume available for the new gas composition. The inner volume of the fuel rod being larger for TRANSURANUS//SCIANTIX, the initial gap

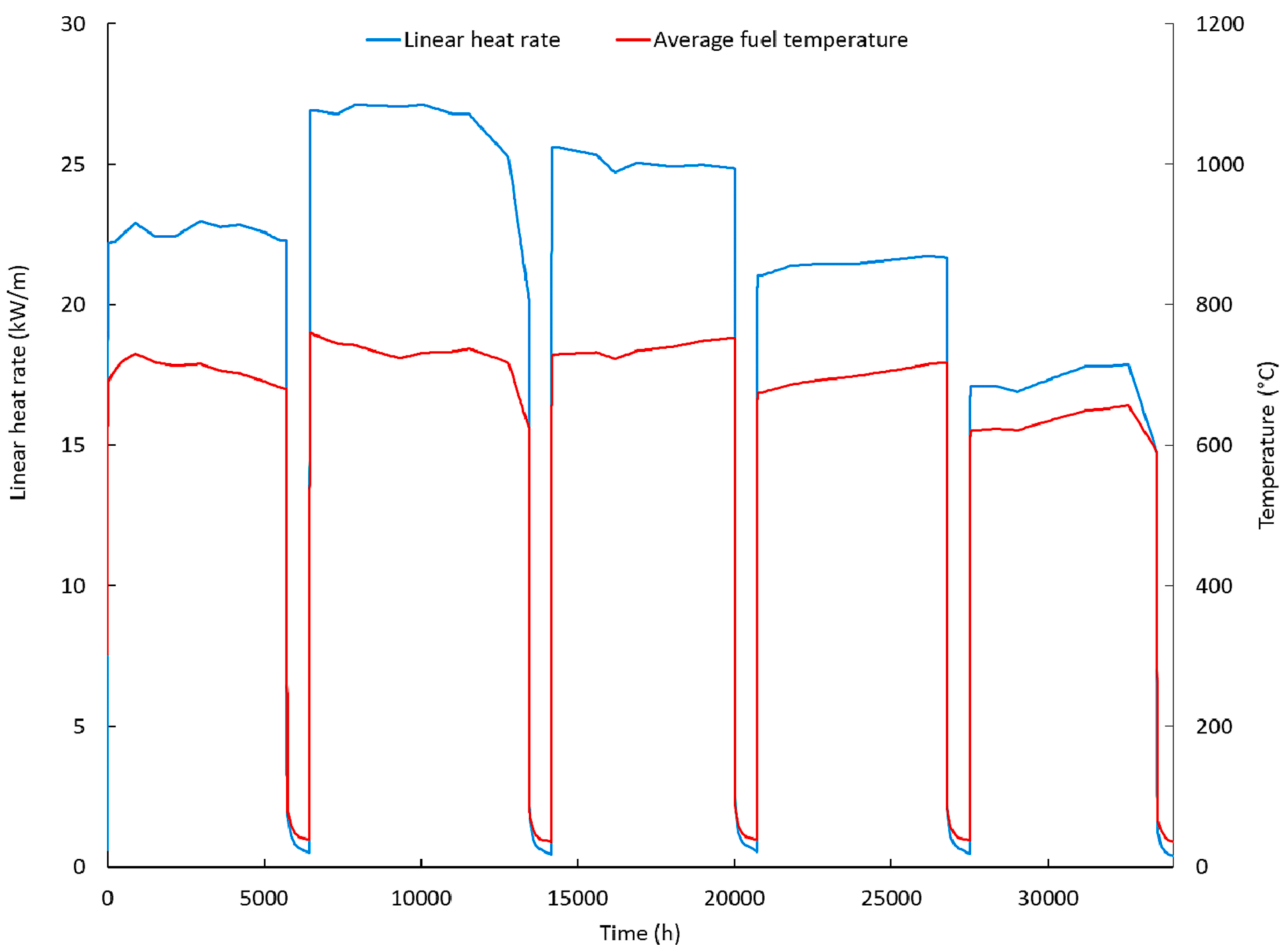

Fig. 3. Input linear heat rate (blue line) and calculated average fuel temperature (red line), of the IFA-650.10 base irradiation phase, simulated with the TRANSURANUS code (FUMAC-TECDOC).

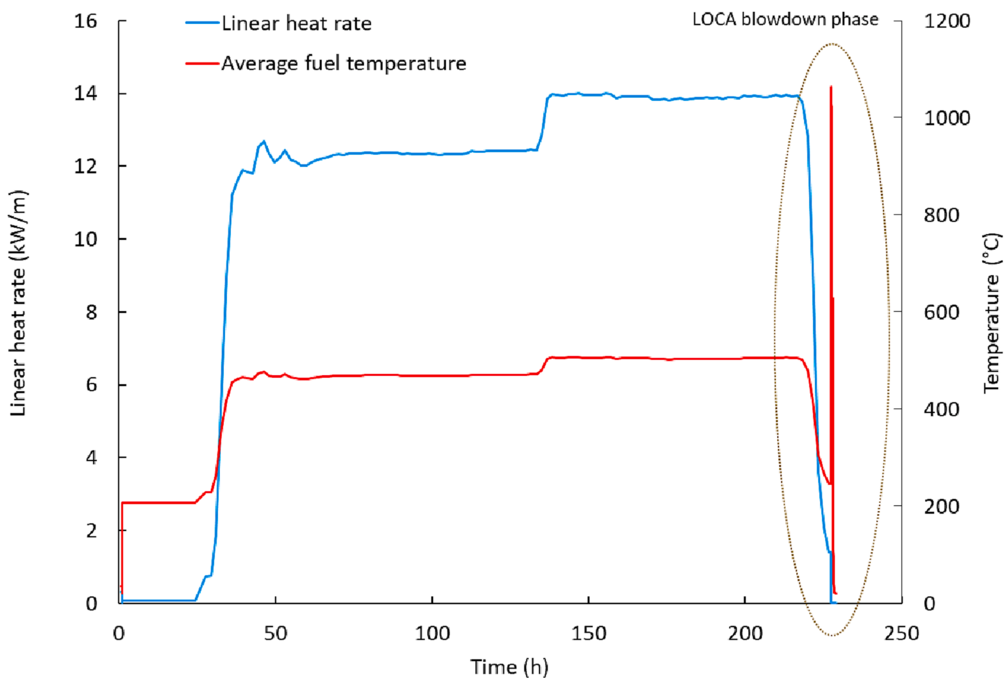

Fig. 4. Enlargement of the transient history for the IFA-650.10 test fuel rod, simulated with the TRANSURANUS code. The LOCA blowdown phase is enclosed in the oval shape. (FUMAC-TECDOC).

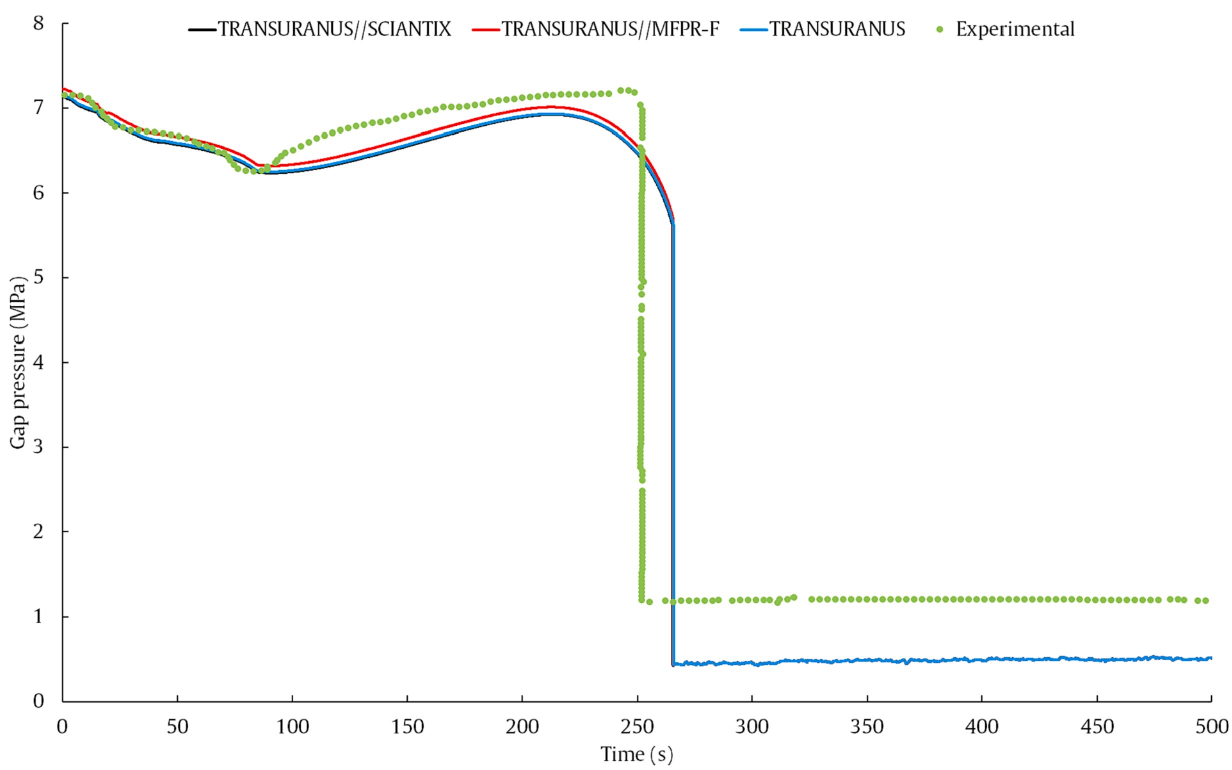

Fig. 5. Comparison of experimental fuel rod internal pressure after the blowdown of the IFA-650.10 test, and calculations of the different TRANSURANUS versions.

pressure is lower, and the same holds for TRANSURANUS and TRANSURANUS//MFPR-F. Details of the integral results obtained at the end of the base irradiation with the three codes are shown in Table 2.

The *meso*-scale codes SCIANTIX and MFPR-F do not significantly affect the burst time predicted by the TRANSURANUS standalone code, i.e., 265 s after the start of the blowdown, whereas the experimental data was at 249 s. Indeed, the gas composition at the end of the LOCA test is always dominated by the rod filling gases helium and argon. As it is reported in Table 3, the concentration of released FGs in the rod free volume at the end of the LOCA test remains below the 1%, therefore their impact on the gap pressure, and ultimately on the burst time, is negligible. The differences on the expected burst time are so minor (under one second) that it is difficult to consider a well-defined phenomenon rather than mere numerical reasons.

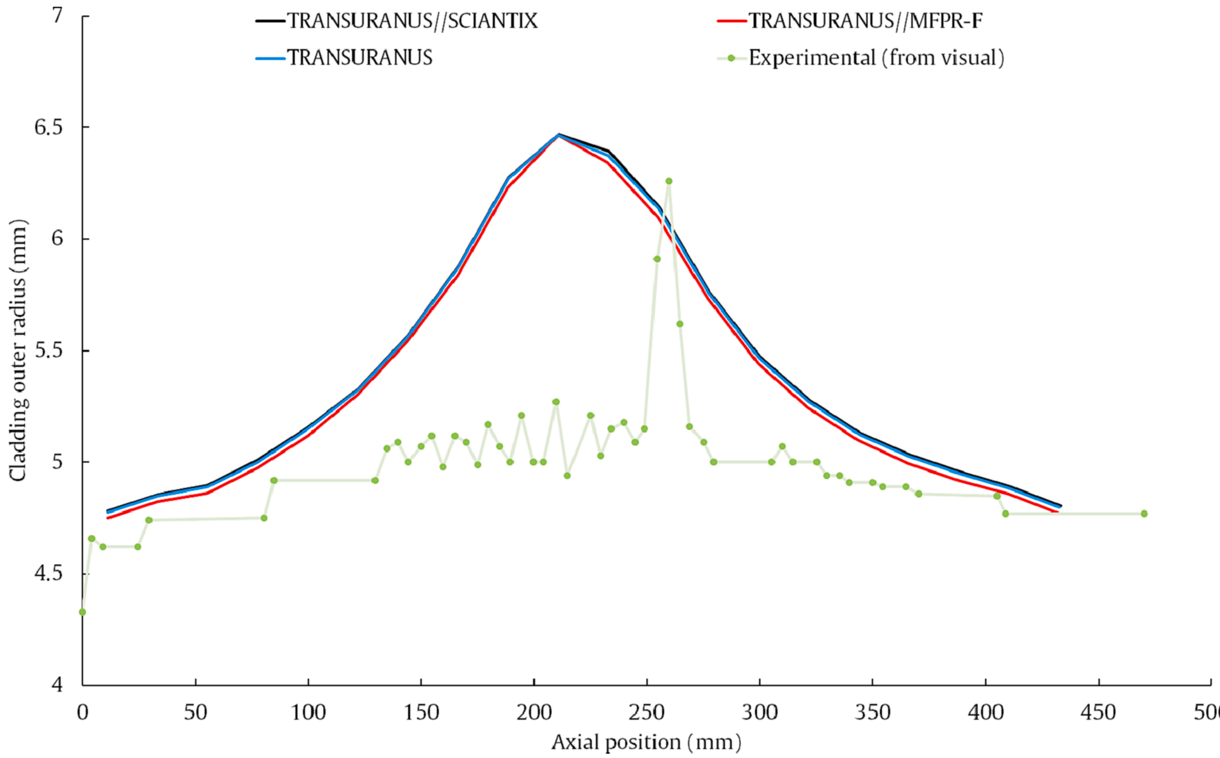

Fig. 6. Comparison of the measured cladding outer radius after the blowdown of the IFA-650.10 test, and calculations of the different TRANSURANUS versions.

Table 2
Results at the end of the base irradiation.

	TRANSURANUS	TRANSURANUS// SCIANTIX	TRANSURANUS// MFPR-F
FGR at the end of the base irradiation (%)	2.55	4.83	0.185
Fuel axial elongation (%)	0.87	1.17	0.93
Cladding axial elongation (%)	0.37	0.49	0.93
Cladding outer radius at burst slice (mm)	4.746	4.753	4.732

FGR due to fuel fragmentation and pulverization may occur in the rim zone of the fuel during a LOCA transient. This contribution is not yet considered in the version of TRANSURANUS considered, nor in SCIANTIX and MFPR-F. Inclusion of this additional contribution to the FGR during the LOCA transient may help to anticipate the calculated burst time by increasing the gap pressure (Bianco et al., 2015).

Fig. 6 shows the cladding profilometry at end of the LOCA transient, compared with the experimental data from PIE. The standalone TRANSURANUS versions describe the single ballooning, but its axial location is higher than the experimental one, as it was obtained in the FUMAC project. Discrepancies with the measured cladding profilometry are ascribable to the 1.5D discretization of the fuel rod, which poorly reproduce axial phenomena, to uncertainties in thermal boundary conditions applied to the outer surface of the cladding, derived from the SOCRAT code (FUMAC-TECDOC; Kiselev, 2016), and lastly due to modelling choices, e.g., use of the small strain approximation.

As in the previous discussion regarding the predicted gap pressure, the calculated outer cladding is not appreciably affected by the FGR

Table 3
Results at the end of the LOCA test.

	TRANSURANUS	TRANSURANUS// SCIANTIX	TRANSURANUS// MFPR-F
FGR at the end of the LOCA test (%)	2.6	6.8	0.2
Transient FGR during blowdown phase (%)	0.0082	1.2	0.0066
Gas composition in the fuel rod free volume (%)	Ar (94.957%) + He (4.997%) + FG (0.46%)	Ar (94.17%) + He (4.95%) + FG (0.88%)	Ar (94.997%) + He (4.999%) + FG (0.004%)
Burst time (s)	265.764	265.276	265.722
Cladding outer radius at burst slice (mm)	6.466	6.468	6.467

predictions of both SCIANTIX and MFPR-F. The differences found in the cladding radius calculated by the three codes are again attributable to the initial conditions, prior refabrication and test. That is, the cladding radius calculated during the base irradiation is different in the three codes (see Table 2) and since it is not modified within the restart option, it influences the cladding radius at the end of the test.

Lastly, Fig. 7 shows the FGR occurring during the LOCA transient, calculated with TRANSURANUS, TRANSURANUS//SCIANTIX and TRANSURANUS//MFPR-F. Although, the impact of the predicted FGR remains negligible in the estimation of burst time and cladding profilometry, it is important to be able to estimate the FGR occurring during LOCA experiments (e.g., to catch the well-known large FGR at high burnup regime (Khvostov, 2022; FUMAC-TECDOC)). Among the three codes, Fig. 7 shows that TRANSURANUS coupled with SCIANTIX predicts the larger transient FGR. The reason why SCIANTIX predicts a large

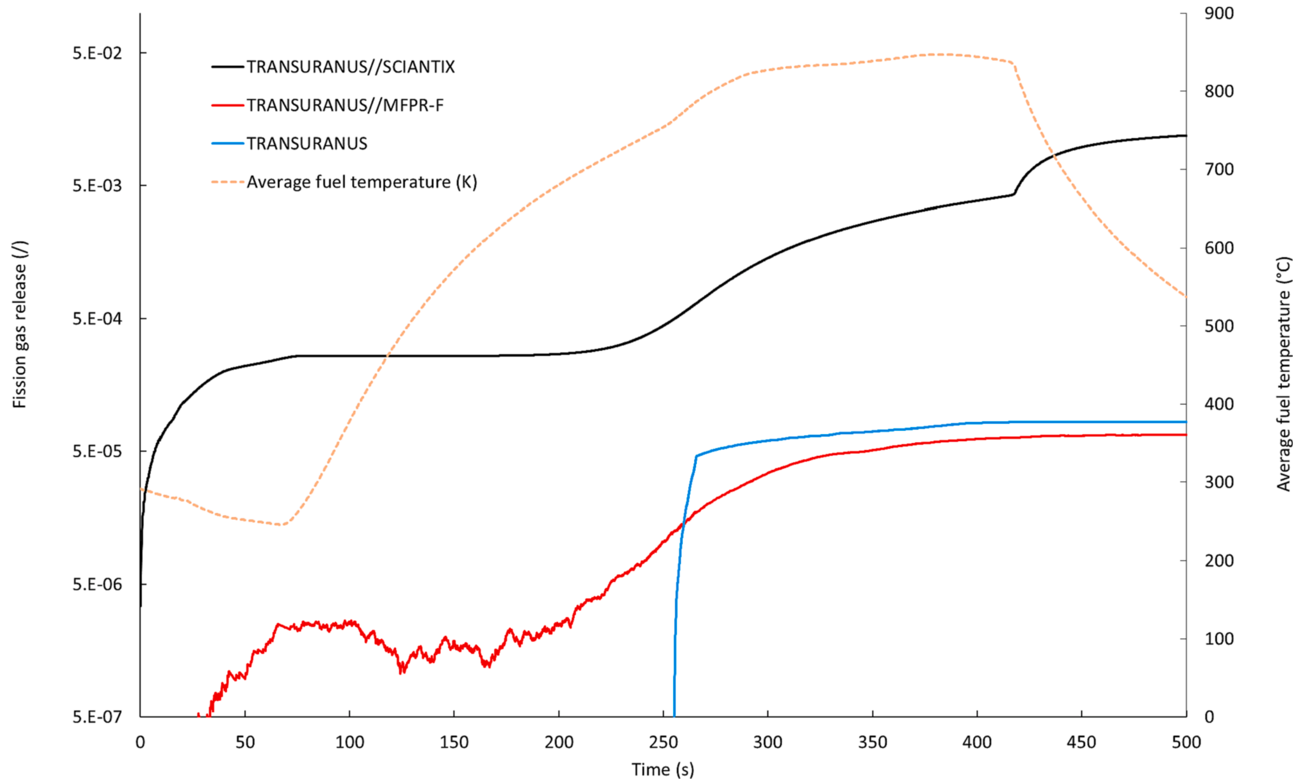

Fig. 7. Comparison of transient FGR predicted during the blowdown phase by TRANSURANUS//SCIANTIX (black line), the TRANSURANUS//MFPR-F (red line) and TRANSURANUS standalone (blue line).

FGR with respect to TRANSURANUS is related to the description of the grain-boundary bubble behaviour and has been discussed in previous works (Zullo et al., 2022). Most of the gas released comes from the grain boundaries, driven by the fuel temperature during the LOCA transient. After the blowdown, the sudden decrease of the fuel temperature accounts for a final increase in the release due to the modelled micro-cracking of the grain boundaries.

4. Conclusions and future perspectives

This work constitutes a first step towards improving the predictions of FGR from nuclear fuels under LOCA accident conditions, by exploiting the conventional FPC TRANSURANUS coupled with mechanistic *meso*-scale modules MFPR-F and SCIANTIX. The main outcomes of this work can be summarised as follows:

- The coupling between TRANSURANUS and the mechanistic *meso*-scale modules for FG/FP behaviour SCIANTIX and MFPR-F has been pursued and assessed against the experimental test IFA-650.10, representative of a LOCA scenario.
- The calculations of the standalone TRANSURANUS version are coherent with calculations of TRANSURANUS coupled with the *meso*-scale modules, for IFA-650.10. In other words, the *meso*-scale codes SCIANTIX and MFPR-F do not alter the TRANSURANUS cladding failure predictions, in line with the outcome of the FUMAC project for the IFA-650.10 case.
- The coupled-code versions can be applied to both normal operation conditions, as well as subsequent accident scenarios without convergence or cliff-edge effects. Therefore, the final versions of the coupled codes turn out to be ready for further simulations of accidental conditions (e.g., additional LOCA simulations).

Up to date with recent modelling trends towards more refined multi-scale and multi-physics descriptions of the fuel rod behaviour, the coupling of validated integral thermo-mechanical FPCs with external mechanistic modules, affords several advantages. These advantages include the potential to describe, at the scale of the fuel grain, fundamental phenomena that impact the overall FPC calculations. Among the phenomena related to the behaviour of inert fission gases, chemically active fission products, as well as their interaction with the fuel matrix microstructure, are of great interest. One can thus reap the benefits from the independent developments made in the *meso*-scale codes and seize the opportunity to improve simulations of high-burnup fuels under accident conditions. Future perspectives of concern for current code coupling activities and application, and for the development of *meso*-scale modules improving integral fuel rod simulations, are:

- The inclusion in mechanistic modules of models to describe high burnup phenomena such as fuel fragmentation, transfer, and dispersal, to enhance rod internal pressure calculations, when significant release of fission gas occurs, complemented with uncertainty and sensitivity analysis.
- The application of coupled code systems to accidental tolerant fuels (ATFs), e.g., U_3Si_2 or Cr_2O_3-doped UO_2 fuel.
- The inclusion of additional phenomena in the TRANSURANUS//MFPR-F coupling (solid swelling, thermal conductivity degradation), based on MFPR-F modelling for fuel chemistry and oxygen redistribution in the pellet. This would allow in particular to consider defective fuel rod, subjected to an oxidizing gap atmosphere.

CRediT authorship contribution statement

G. Zullo: Conceptualization, Methodology, Software, Validation, Writing – original draft, Writing – review & editing, Visualization. **D. Pizzocri:** Conceptualization, Methodology, Software, Writing – review & editing. **L. Luzzi:** Writing – review & editing, Funding acquisition, Supervision. **F. Kremer:** Conceptualization, Software, Validation, Writing – review & editing. **R. Dubourg:** Conceptualization, Writing –

review & editing, Supervision. **A. Schubert:** Software, Writing – review & editing. **P. Van Uffelen:** Conceptualization, Methodology, Software, Writing – original draft, Writing – review & editing, Funding acquisition, Supervision.

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

The authors do not have permission to share data.

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