APPLICATION OF INTEGRATED RELAP5-TRANSURANUS APPROACH TO A RIA BENCHMARK EXERCISE INCLUDING UNCERTAINTY AND SENSITIVITY ANALYSIS

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ABSTRACT

A Reactivity Initiated Accident (RIA) Fuel Codes Benchmark was organized by the OECD/NEA Working Group on Fuel Safety. While the phase-I of the exercise focused on the analysis of power pulse tests performed on research reactors, the phase-II dealt with the benchmarking and comparison of participants' modelling approaches: (task 1) to the analysis of several idealized RIA cases, and (task 2) with sensitivity analysis and uncertainty quantification (through the analysis of one particular RIA case). This paper describes the work performed by NINE as one of the participants to phase-II, and particularly on task 2. Such work involved the integrated use of two different codes, namely RELAP5 and TRANSURANUS for the thermal hydraulic and the fuel performance parts of the analysis respectively, the integration consisting in an off-line one-way sequential coupling. According to the benchmark specifications, the uncertainty analysis was performed by adopting a Monte Carlo statistical approach, requiring 200 runs with a number of uncertain input parameters randomly sampled from a specified Gaussian distribution, and by applying a 95/95 statistics to the selected output variables. Moreover, the sensitivity analysis was performed by calculating the Spearman's rank correlation coefficients of specified output variables versus specified input parameters. The whole analysis process was handled through a Python-based "Statistical RELAP5-TRANSURANUS" (StaRT) coupled analysis programme developed on purpose. StaRT takes care of input parameter sampling, update of RELAP5 and TRANSURANUS input decks, post-processing of both codes' results, uncertainty and sensitivity analyses. All the results produced at key steps of the process are stored in a single HDF5 file. StaRT turned out to be an effective tool for the purposes of the benchmark as well as for future applications to similar studies.

1. INTRODUCTION

The assessment of fuel performance during nuclear reactor normal and off-normal conditions is a crucial aspect of nuclear reactor safety analysis, as it directly concerns the effectiveness of the first two of the fundamental safety barriers against the release of radioactive substances during accidental scenarios, i.e. the fuel and its cladding. Understanding and modelling the fuel behavior is a particularly complex problem, because it involves several physics (neutronics, coolant thermal-hydraulics, thermo-mechanical and chemical behavior of materials – including effects of neutron irradiation, fission products decay and dispersion, etc.) and closely-coupled interactions between them, along with a large number of specific phenomena and processes to be accounted for.

Best estimate (BE) computer codes are nowadays available (such as TRANSURANUS, FRAPCON / FRAPTRAN, BISON, SCANAIR, etc.), which can simulate the fuel behavior in a variety of operating conditions, relying on sets of models able to deal with many of the phenomena involved, and possibly including limited capabilities to account for the interactions with neutron physics and coolant thermal-hydraulics. Such tools, in principle, can provide detailed and accurate information on the fuel behavior (e.g. on fuel and clad deformation and stress conditions, on temperature radial distribution across fuel rod, on distribution of fission products, etc.) However, Verification and Validation (V&V) efforts are still necessary in order to demonstrate the codes' capabilities for all situations of interest and quantify the accuracy of their predictions. Moreover, Uncertainty Quantification (UQ) methods need to be developed and assessed in order to allow consistent application of such BE tools in Nuclear Power Plant (NPP) safety analysis frameworks. Furthermore, a realistic modelling also requires that the multi-physics nature of the problems be adequately taken into account: this can be obtained through "coupling" of fuel performance codes with neutronics and thermal-hydraulics codes (which in turn brings further V&V issues to deal with).

A relatively recent picture of the state-of-the-art as to reactor safety-related multi-physics simulations, including fuel behaviour analysis, is constituted by a special issue on "Multi-Physics Modelling of LWR Static and Transient Behaviour" published in October 2015 in Annals of Nuclear Energy (see, for example, [1] to [4]).

Concerning UQ of fuel performance codes, to the authors' knowledge most of current efforts are limited to extensions of the GRS method (see, for instance, [5]), which suffers from some limitations, particularly its being prone to user-effect, as well as the need for extensive engineering judgment to characterize and prioritize the uncertain input parameters from which the results' uncertainty propagates. To overcome such limitations, R&D activities (not covered in the present paper) are currently in progress at NINE to develop alternative UQ methods for fuel analysis, based on adjoint sensitivity analysis and including data adjustment and assimilation; such approach is the same as that described in [6] for TH code analysis.

This paper relates to work performed in the frame the second phase of the "RIA Benchmark" organized by the OECD/NEA Working Group on Fuel Safety (WGFS).[1] The benchmark exercise dealt with UQ of the results of fuel performance codes applied to a selected idealized case, i.e. a Reactivity Initiated Accident (RIA). Such idealized case consists of a 10 cm long PWR fuel rodlet (with slightly enriched fresh UO2 fuel, Zircaloy-4 cladding, closed fuel-clad gap, filled with 20 bar Helium at room temperature), cooled by a 4 m/s water flow at 280 °C and 15.5 MPa, subjected to a triangular power peak (1 MW maximum power, 15 ms full width at half maximum).

The participants were requested to perform an UQ analysis by a Monte Carlo statistical method running a fixed number of code simulations with randomly sampled values for a prescribed set of input parameters. Sensitivity analysis for a given set of output variables was requested as well.

The fuel performance code used by the authors of the present paper is TRANSURANUS (TU, [7]). Such code has thermal-hydraulic (TH) modelling capabilities, which however are rather limited and do not allow appropriately accounting for complex TH phenomena occurring during most accidental scenarios. Therefore a simulation strategy was applied which involves a combined TH / fuel performance analysis: namely, for each "case" a standalone TH simulation is performed by the RELAP5 code (R5 in the following), then a TU simulation is setup an run with boundary conditions derived from the TH simulation results. In other words, it is an external, sequential, one-way "coupling" of the two codes.

The TU code has the embedded capability to perform Monte Carlo statistical analyses; however, the random sampling can only be operated on a limited set of input variables, which does not include all the variables that the Benchmark specified. Due to such limitation, the option of using the statistical version of TU was discarded. On the other hand, even for standard TU runs there are a few specified variables which cannot be defined by the user in an input deck. Overcoming such limitation required implementing modifications in the code sources and recompiling the code.

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[1] Information on the WGFS can be found on the website: https://www.oecd-nea.org/nsd/csni/wgfs/.

Further customization of the TU code was necessary to allow the efficient "extraction" of the entire set of target variables from the simulations results for UQ and sensitivity analysis purposes.

As mentioned above, the overall study involved running many R5/TU coupled calculations and performing all the related pre- and post-processing tasks, including the random sampling of the specified input variables, the preparation of both codes input decks, the extraction of relevant output variables from both codes' results (and R5-to-TU transfer), the final QU and sensitivity analysis. All those tasks obviously require an automated tool, both for efficiency reasons and to limit error-prone user operations. The Python-based "Statistical RELAP5/TRANSURANUS Analysis Tool" (StaRT), was thus developed for such purposes and utilized for the benchmark activity.

2. THE RIA BENCHMARK PHASE II ACTIVITY 2

The Phase I of the RIA Benchmark dealt with the assessment and comparison of fuel performance core capabilities to simulate RIA scenarios; the recommendation of performing such exercise had been an outcome of the technical workshop on "Nuclear Fuel Behaviour during Reactivity Initiated Accidents" organized by the OECD/NEA in September 2009. The exercise allowed assessing the performances of different codes in relation to various modelling aspects, such as the thermal behaviour of the fuel and of the cladding, the mechanical behaviour of the cladding, the fission gas release, the prediction of failures etc., the involved phenomenology being noticeably complicated by the presence of boiling of the coolant. It was concluded (ref. [8]) that, owing to the scatter observed in the results obtained by different codes, a deeper understanding of the differences between the different modelling approaches and of the respective performances was necessary. Such task would have required a further assessment step, to be performed of a simpler, more fundamental, exercise: this was addressed by the First Activity of a Phase II of the RIA Benchmark, launched early in 2014 (see specifications in [9], and [10]).

Moreover, it was concluded from the Phase I that also an assessment of the uncertainty of the results was to be performed, along with a sensitivity analysis of the results to the input parameters: that task was dealt with by the Second Activity of the RIA Benchmark Phase II (see specifications in [11]). The present paper addresses the Second Activity only. A summary of the outcomes of that benchmark exercise is included in [12].

The key specifications for the exercise are summarized hereafter.

- The reference case to be simulated is "Case 5" of the First Activity [9]. This case is one of those addressing the "PWR thermal-hydraulic assessment".
  - o The clad inner diameter is equal to 8.26 mm. The fuel-clad gap is assumed closed; a no-slipping condition is assumed between cladding and fuel.
  - o PWR nominal conditions are assumed for the coolant (Pcool = 155 bar; Tcool = 280 °C; Vcool = 4 m/s; channel radius = 7.5 mm). A maximum power equal to 1100 kW is reached, so as to achieve boiling conditions. The helium pressure inside the fuel rod is 20 bar at 20 °C.
  - o A triangular power pulse is imposed, with 30 ms of Full Width at Half Maximum (FWHM), starting from zero power. Flat radial and axial profiles are assumed.
  - o Fuel and cladding are initialized at room temperature and zero power. The coolant is initialized at room temperature and pressure and at Vcool.
  - o The coolant temperature and pressure rise to the nominal values in 50 s.
  - o The power pulse occurs between 100.00 s and 100.06 s, the power peak thus being at 100.03 s.
  - o The overall transient lasts 200 s.
- A well-established UQ methodology, based on input uncertainty propagation (so-called GRS method, see [13]), is proposed, which all participants are requested to use.
  - o A set of 19 potentially influential input parameters, independent on each other, is selected. A probability density function (pdf) is defined for each variable to quantify the related uncertainty, based on experience and engineering judgement. Such information is summarized in Table I.

o The input uncertainties are propagated through the code by performing Monte Carlo calculations: many simulations are run, each characterized by a different set of input parameters randomly sampled from the respective pdfs. The number of calculations to perform (in addition to the "reference" run) is set to 200 for all participants.

The results are statistically analysed: means and variances of the specified output variables (time-dependent quantities reported in

o Table II, plus their maximal values and their times-to-maximum, and the time to quenching) are determined, along with the related cumulative distribution functions, in order to obtain lower and upper uncertainty bands. The confidence interval defined by the 5% and the 95% percentiles is focused on, with a confidence level higher than 95%.

- A sensitivity analysis based on the statistical runs is requested too, in order to identify the most influential input parameters. In particular, it is requested to calculate correlation coefficients2 relating the specified set of output variables to the uncertain input parameters. The sensitivity analysis focuses on the values that the selected variables (the same as those of the uncertainty analysis) assumed at the five instants defined in Table III, as well as the maximal values. A ranking of the importance of each sensitivity parameter is requested too (by three arbitrarily defined levels: High, Medium and Low).

Table I. Uncertain input parameters for uncertainty analysis, as per Benchmark specifications (adapted from Table 2-1 of [11]).

| # | Input uncertainty parameter | Distribution | | | | | Code |
		Mean	Std. Dev.	Type	Lower bound	Upper bound	
1. fuel rod manufacturing tolerances							
1	Cladding outside diameter (mm)	9.40	0.01	Normal	9.38	9.42	TU
2	Cladding inside diameter (mm)	8.26	0.01	Normal	8.24	8.28	TU
3	Fuel theoretical density (kg/m3 at 20 °C)	10970	50	Normal	10870	11070	TU
4	Fuel porosity %	4	0.5	Normal	3	5	TU
5	Cladding roughness (µm)	0.1	1.	Normal	$10.^{-6}$	2.	TU
6	Fuel roughness (µm)	0.1	1.	Normal	$10.^{-6}$	2.	TU
7	Filling gas pressure (MPa)	2.0	0.05	Normal	1.9	2.1	TU
2. Thermal hydraulic boundary conditions							
8	Coolant pressure (MPa)	15.500	0.075	Normal	15.350	15.650	R5
9	Coolant inlet temperature (°C)	280	1.5	Normal	277	283	R5
10	Coolant velocity (m/s)	4.00	0.04	Normal	3.92	4.08	R5
3. Core power boundary conditions							
11	Injected energy in the rod (Joule)	30000	1500	Normal	27000	33000	R5
12	Full mid height width (ms)	30	5	Normal	20	40	R5
4. Physical Properties/Key models							
13	Fuel thermal conductivity model (Mult. Coef.)	1.00	5%	Normal	0.90	1.10	TU
14	Clad thermal conductivity model (Mult. Coef.)	1.00	5%	Normal	0.90	1.10	TU
15	Fuel thermal expansion model (Mult. Coef.)	1.00	5%	Normal	0.90	1.10	TU
16	Clad thermal expansion model (Mult. Coef.)	1.00	5%	Normal	0.90	1.10	TU
17	Clad Yield stress (Mult. Coef.)	1.00	5%	Normal	0.90	1.10	TU
18	Fuel enthalpy / heat capacity (Mult. Coef.)	1.00	1.5%	Normal	0.97	1.03	TU
19	Clad to coolant heat transfer ((Mult. Coef. - Same Coef. applied for all flow regimes)	1.00	12.5%	Normal	0.75	1.25	R5

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2 Such as: Linear (Pearson's) Simple Correlation Coefficient (SCC), Partial Correlation Coefficient (PCC), Spearman's Rank Correlation Coefficient (RCC); Partial Rank Correlation Coefficient (PRCC).

Two open-access UQ and sensitivity analysis tools were proposed by the Benchmark organizers, namely DAKOTA (Design Analysis Kit for Optimization and Terascale Applications code, developed by the Sandia National Laboratory [14]) and SUNSET (Sensitivity and UNcertainty Statistical Evaluation Tool, developed by the Institut de Radioprotection et Sûreté Nucléaire, IRSN [15]). However the use of those two tools was not mandatory and the participants were allowed to resort to different tools, provided that the same methodology was adopted.

Table II. Output parameters for uncertainty analysis (adapted from Table 2-2 of [11]).

#	Parameter	Unit	Description
1	DHR	cal/g	Variation of radial average enthalpy with respect to initial conditions of the transient in the rodlet as a function of time (at z=h/2) Note that: DHR(t=0)=0
2	TFC	°C	Temperature of fuel centreline as a function of time (at z=h/2)
3	TFO	°C	Temperature of fuel outer surface as a function of time (at z=h/2)
4	TCO	°C	Temperature of clad outer surface as a function of time (at z=h/2)
5	ECTH	%	Clad total (thermal + elastic + plastic) hoop strain at the outer part of the clad as a function of time (at z=h/2)
6	ECT	mm	Clad total axial elongation as a function of time
7	EFT1	mm	Fuel column total axial elongation as a function of time
8	SCH	MPa	Clad hoop stress at outer part of the clad as a function of time (at z=h/2)
9	RFO	mm	Fuel outer radius as a function of time (at z=h/2)

Table III. Times for sensitivity analysis (adapted from Table 2-3 of [11]).

Time parameters	t_1	t_2	t_3	t_4	t_5
Definition	Beginning of power pulse	Time of maximum power pulse	End of power pulse	101s	End of calculation
Value	100.000s	between 100.020s and 100.040s	between 100.050s and 100.070s	101.000s	200.000s

3. THE ADOPTED ANALYSIS PROCEDURE

As mentioned above, the adopted methodology consists of running Monte Carlo "coupled" R5/TU simulations of the specified RIA idealized scenario and performing related uncertainty & sensitivity analysis, through an automatized process.

The intention of the multi-physics analysis is to take into account the influence of coolant-cladding heat transfer (through the various regimes experienced during the transient) on the fuel thermo-mechanical behavior; on the other hand, the simplifying assumption is made that the fuel thermo-mechanical changes do not affect the thermal-hydraulics. This leads to an off-line one-way coupling approach ("coupling" being thus intended in a loose sense).

The first step of the statistical analysis consists of the uncertain input parameters sampling, as described above. Then a series of coupled R5/TU simulations are run: one is the reference case (based on nominal values for all input parameters) and all other runs have randomly varied input according to the above sampling.

Each coupled analysis consists of:
- R5 standalone run for the entire duration of the transient (200 s);
- extraction of selected R5 time-dependent results and incorporation into TU simulation input as boundary conditions (BC);
- TU standalone run for the entire duration of the transient (200 s).

The R5 results transferred to TU are:
- linear power;
- coolant pressure;
- clad outer temperature at each axial node ("slice" in TU jargon);
- upper plenum temperature.

Clearly, the clad-to-coolant heat-transfer is more accurately dealt with by R5 than by TU, thus one would directly impose the cladding temperature predicted by R5 as a BC to TU. However, what TU expects as a BC is coolant temperature (the heat transfer coefficient being either user-specified or estimated by own models). To cope with that, the R5 cladding temperature was actually imposed as a dummy coolant temperature BC to TU, along with an infinite heat transfer coefficient (this is a TU feature which allows bypassing its internal TH routines).

All uncertain input variables (Table I) specified in the Benchmark are accounted for in the random sampling and in R5 and TU runs setup; the rightmost column of the same table also indicates which input parameters are relevant to which code. Likewise, all specified output variables (Table II) are extracted and processed.

As mentioned above, TU code customization was needed for these purposes. In fact:
- The standard version of TU does not envisage user's input for parameters #3 and #13-18 of Table I, as they are automatically handled by the code through its embedded models for fuel and clad materials, once the latter have been selected by the user; so it was necessary to implement multiplying factors through which those quantities are time by time modified according to the Monte Carlo sampling.
- A specific post-processing routine was coded into TU in order to "extract" all specified output variables in a ready-to-use format.

The custom TU solver executable was built for Microsoft Windows 7-64bit by a GCC Fortran compiler under "Eclipse" Integrated Development Environment (IDE) combined with "Cygwin" UNIX-like environment for Windows. Verification tests were performed in order to check the correct implementation of the modifications.

The procedure ends with UQ and sensitivity analysis by statistical processing of all selected results:
- order statistics is performed to obtain lower and upper uncertainty bands (5% and 95% percentile respectively);
- Spearman's Rank Correlation Coefficients are calculated for all output variables evaluated at relevant times reported in Table III (as well as for their maximal values).

All the above process was handled by StaRT, which is described in the following section.

3.1. The Statistical RELAP5/TRANSURANUS Analysis Tool (StaRT)

StaRT is a software tool, implemented through Python subroutines, which automatically performs the statistical coupled R5/TU simulations and the uncertainty and sensitivity analysis, and generates the output requested for the RIA Benchmark – Phase II – Activity 2.

It is an in-house tool, developed on-purpose for this specific application; with further development efforts its applicability can be made more general. Although well-established existing software such as DAKOTA, SUSA or SUNSET could have been used otherwise (at the expense of some learning time), the development of such simpler and focused tool was preparatory to other R&D programs being planned at NINE, allowed to efficiently deal with the Benchmark commitment, and required limited efforts.

Figure 1 shows a sketch of the overall analysis process, indicating tasks performed by StaRT, tasks performed by the user, and output produced at key steps.

The information to be input by the user consists of:
- pdfs of uncertain input parameters (in terms of nominal value, standard deviation, lower/upper values, assuming that all distributions are normal); number of Monte Carlo runs (N); "seed" for random number generator (for repeatability purposes);
- templates for R5 and TU input setup;
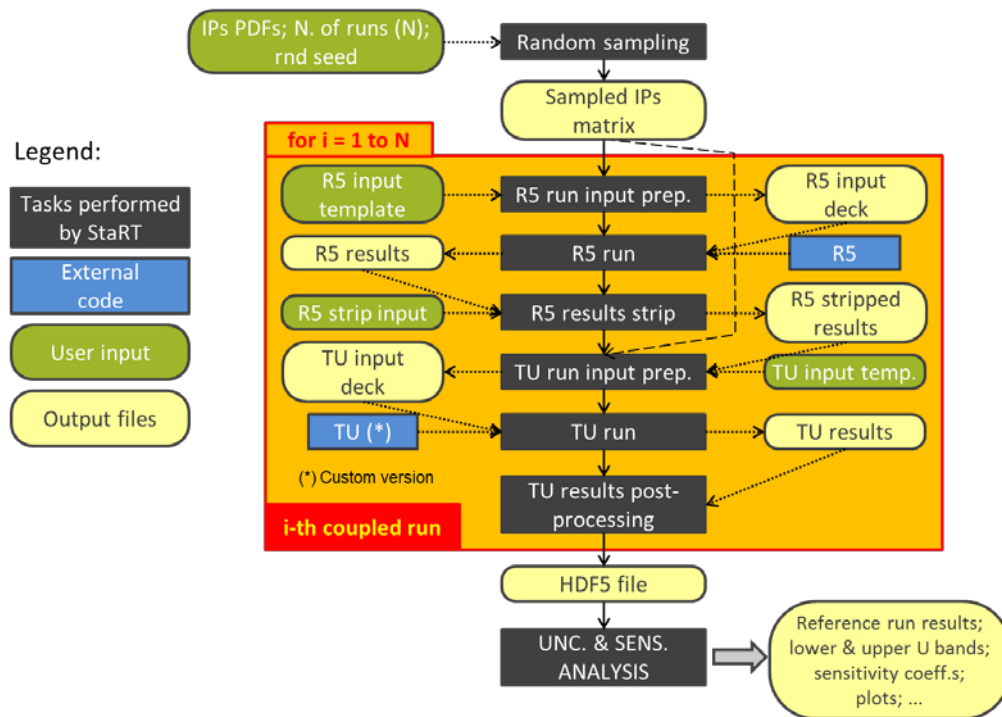- input deck for R5 results extraction (strip).

Figure 1. Overall analysis procedure and StaRT tasks.

The tasks performed by StaRT (and related outputs) are:
- only once (before Monte Carlo runs):
  - random sampling of input parameters → matrix of N x 19 sampled values on an ASCII file
- for each Monte Carlo run:
  - preparation of R5 input (from template + sampling) → input deck on ASCII file
  - execution of R5 solver → R5 results (files in native format)
  - "stripping" of selected R5 results → stripped R5 results on an ASCII file
  - preparation of TU input (from template + sampling + R5 results) → input deck on ASCII file

- o execution of TU solver → TU results (files in native format + custom ASCII files with selected variables for Benchmark purposes)
  - o post-processing of TU results → data stored in a HDF5 file in the form of tables
- only once (after Monte Carlo runs):
  - o uncertainty and sensitivity analysis → further data stored in HDF5 files in the form of tables, and plots

The codes used are:
- RELAP5
- TRANSURANUS, customized from Version 1 Modification 1 Year 2015 (V1M1J15)

StaRT is constituted by a dozen Python routines, sequentially and/or iteratively called by a "master" routine. The entire set of routines counts about a thousand lines of code. Python version 2.7.11, embedded in Anaconda 2.5 suite, was used.
Several modules (i.e. Python libraries) were imported to enhance "base" Python features; in particular:
- *pandas*: provides high-performance data structures and data analysis tools (including interfaces with HDF5 files);
- *numpy*: provides very efficient high-level math functions (e.g. for vector and matrix operations) useful for scientific computing applications;
- *scipy*: based on *numpy*, provides further tools for scientific computing (e.g. statistical functions);
- *matplotlib*: provides efficient and easy-to-use 2D plotting tools;
- *os*: interface with the operating system (e.g. for executing DOS- or UNIX-like commands, like, for instance, launching code solver executables).

Here is a list of some of the key operations that are handled by the Python routines:
- interface to operating system to launch R5 and TU executables and manage related input/output files;
- text handling to update input decks and prepare outputs; reading arrays of results from ASCII files to memory; etc.
- random sampling from normal distributions (by means of an *ad hoc* built-in numpy function);
- aligning all output variables time-histories to the same reference time vector (as per Benchmark specification), performing data interpolation where necessary;
- calculating relevant statistics;
- calculating Spearman's Rank Correlation Coefficients;
- handling HDF5 files.

Concerning the latter item, Hierarchical Data Format files (HDF5) are a powerful means for storing and handling scientific data in a more compact, efficient and portable way than traditional file system-based storing. StaRT writes all key results of a statistical analysis (sampled values; selected R5 and TU results; post-processed results; UQ and sensitivity analysis results) onto a single HDF5 file, which can then be read and browsed with many different tools openly available.

Various Verification tests were performed at several stages of the development of StaRT, in order to verify that interfaces and processing functions had been implemented and were working as intended. When appropriate, functions' outcomes were compared against results from spreadsheet processing for consistency check. Further contribution to the verification process came from the comparison with results from other Benchmark participants: at a first step, such comparison allowed spotting a few bugs in the target variables processing; those issues were then fixed and updated results were submitted.
A more systematic and extended V&V process will have to be performed in the framework of possible StaRT development follow-up activities.

4. BENCHMARK CALCULATIONS

4.1. Setup of R5 and TU Calculations

As explained above, StaRT prepares the input decks for R5 and TU simulations from two template input decks provided by the user at the beginning of the process. "Template" means here a typical input file where certain character strings (a sort of placeholders) replace the numerical fields that must be automatically input by StaRT before each R5/TU coupled run.

The R5 template is a nodalization with the following main features:
- a *pipe* representing the 10 cm long coolant channel (6 nodes, 5 of which correspond to fuel and 1 to rod upper plenum);
- a *time dependent volume*, a *time dependent junction*, and a *branch* upstream of the *pipe*, to apply coolant velocity and temperature as inlet boundary conditions (items #10 and #09 in Table I);
- a *branch* downstream of the *pipe*, representing the upper plenum;
- a *time dependent volume*, to apply coolant pressure as an outlet BC (item #08 in Table I);
- 5 *heat structures*, representing axial slices of fuel rod (UO2 fuel + Zry clad, with closed gap as per specifications); a "fouling factor" is applied on the water-side boundary to alter the self-calculated heat transfer coefficient according to the random sampling (item #19 in Table I);
- a power table, where triangular power pulse is implemented through relevant quantities (times of start, peak and end; peak power) that are calculated by StaRT as functions of sampled values for items #11 and #12 in Table I.

The TU input deck has the following main features:
- PWR UO2 fuel (fresh) and Zry cladding;
- 6 axial slices to model the fuel rod (1 of which is for upper plenum);
- 5 radial coarse zones for fuel + 1 for cladding;
- 15 mesh points for each fuel coarse zone; 10 for cladding;
- number of cracks in the fuel: 0 (this assumption is further discussed below);
- fuel rod geometry: inner and outer fuel radius (0 and #2 in Table I); inner and outer cladding radius (#2 and #1 in Table I); fuel and cladding surface roughness (items #6 and #5 in Table I);
- customized input: items #3 (multiplier for fuel density) and #13-18 (multipliers for: clad and fuel thermal conductivities and expansion coefficients; clad yield stress; fuel heat capacity) in Table I, enabled by an *ad hoc* flag and not existing in standard TU version).

The part related to time-dependent boundary conditions is missing from the template, as it will be directly created by StaRT as soon as the relevant R5 results are available for being transferred to TU.

4.2. Results of Statistical Calculations with UQ and Sensitivity Analysis

Some results of the Monte Carlo R5/TU coupled analysis for the RIA benchmark exercise are shown in Figure 2 and Figure 3, in terms of time trends from reference calculation and lower and upper uncertainty bands obtained from the statistical analysis. All plots are automatically created by StaRT.

As the power pulse occurs, all quantities increase immediately and reach their peak values. Then, what happens in the next 5-10 sec is governed by materials thermal inertia and by cladding-coolant heat transfer regime. In particular, smoothly decreasing trends are observed for several seconds (about 6.5 s in the reference case), during which a boiling heat transfer regime takes place; then temperatures (and other

affected quantities) drop rapidly because of the "quenching" (i.e. the heat transfer regime getting back to subcooled liquid convection)[3].

It is worth noticing that, after the power pulse, the calculated strain conditions of fuel and cladding show quite a different behavior: the former returns to the same conditions as before the power pulse (Figure 3-c and -d), while the latter keeps noticeable residual deformation (Figure 3-a and -b), due to the plasticization induced by hard mechanical interaction with the fuel during the pulse. This also explains the compression stress state predicted in the cladding (Figure 3-e).
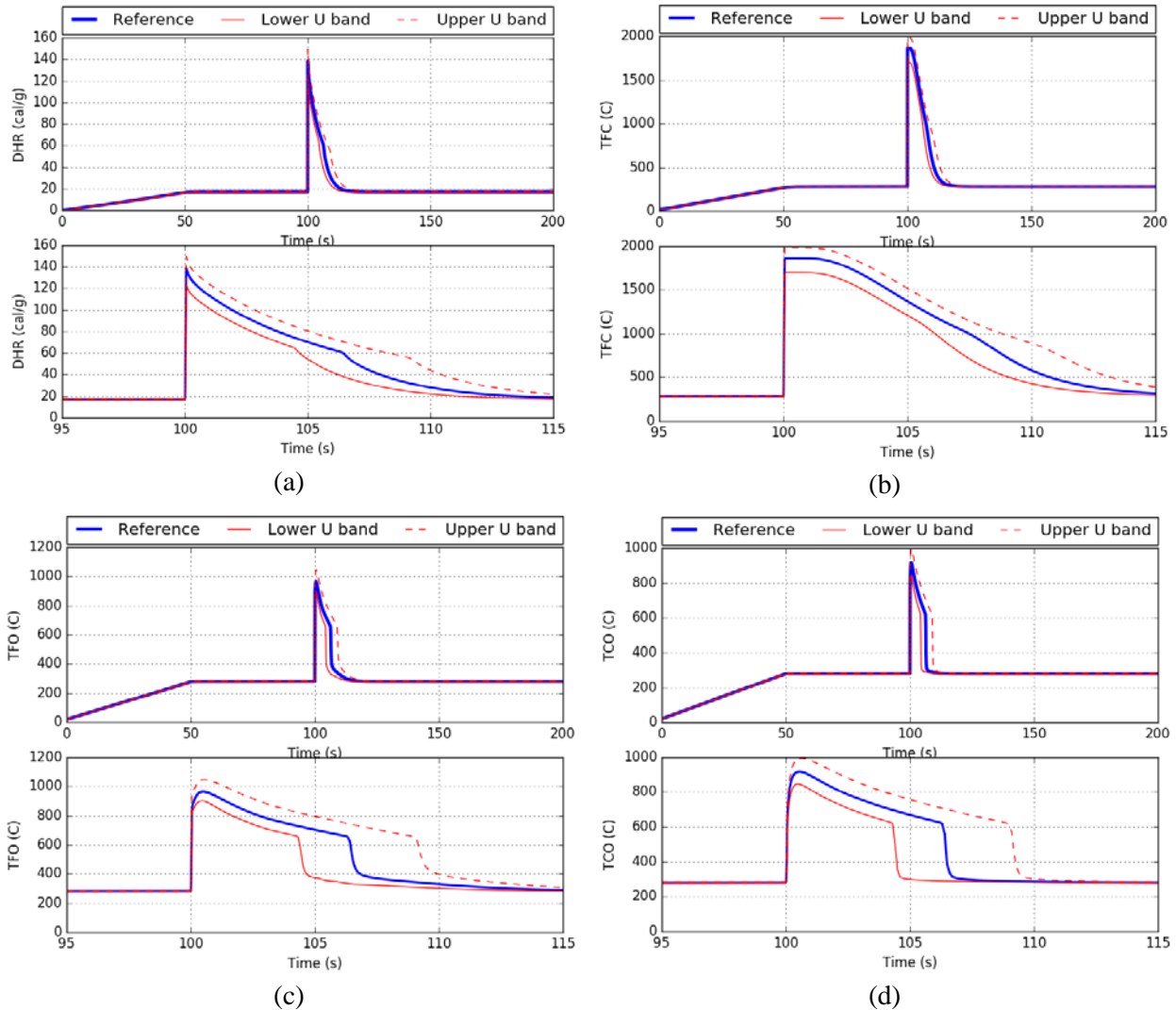

Figure 2. Monte Carlo calculation results: a) time variation of radial average enthalpy; b) fuel centerline temperature; c) fuel outer surface temperature; d) cladding outer surface temperature.

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[3] This is the part of the modelling which supposedly takes advantage of the multi-physics analysis approach. Obviously, a rigorous validation effort would be necessary to confirm such expectation. This aspect is out of the scope of the benchmark activity, which rather focuses on code-to-code comparison.
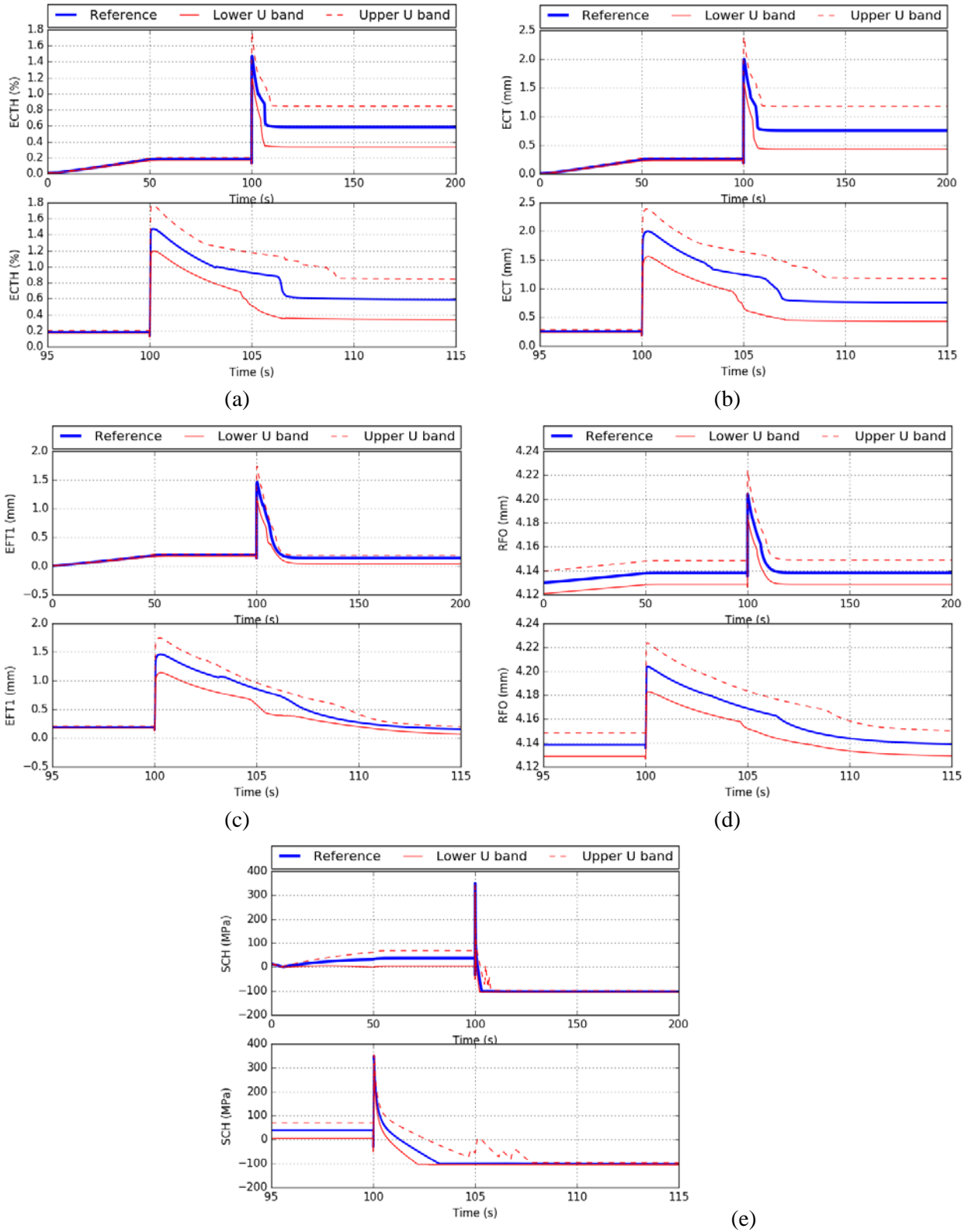
Figure 3. Monte Carlo calculation results: a) outer clad total hoop strain; b) clad total axial elongation; c) fuel total axial elongation; d) fuel outer radius; e) clad hoop stress.

The uncertainty bands obtained show significant dependence of the results on the uncertain input parameters. Moreover, for all shown results the uncertainty bands have the same qualitative trends as the reference curves, with only one exception: the clad stress upper band shows a jagged trend during the quench phase, which can probably be explained by certain combinations of sampled input parameters such that a discontinuous mechanical interaction between fuel and cladding is still taking place. Preliminary results (presented during Benchmark meetings) from the analyses performed by all participants had shown significant dispersion, in term of both reference trends and uncertainties. The present results are qualitatively and quantitatively similar to those of other participants.
They also showed discrepancies worth of further investigations.
Such benchmark-related evaluations, however, are outside the scope of the present paper and will rather be thoroughly discussed and published by the WGFS.

A critical aspect of the analysis performed is the modelling of the fuel "cracking" and of the consequent effects on mechanical properties. TRANSURANUS utilizes a correlation that estimates the Young modulus of the fuel also as a function of the "number or cracks", a parameter which is to be input by the user and is typically set to 4-6 for normal operating conditions (the larger the number of cracks, the smaller the elasticity constant). However, the fuel may show quite a different behavior during a rapid power excursion than in slow transients, which the currently available modeling is not able to account for. Moreover, while fresh fuel is assumed in the benchmark exercise, a zero-crack assumption (made also in the present analysis) becomes invalid as soon as the power peak occurs.

A separate study was performed to demonstrate the sensitivity of TU results on the number of cracks, using the benchmark exercise as a case test. Namely, several TU standalone simulations were run setting different numbers of crack (0, 2, 4 and 6). In addition, a calculation was run with zero cracks until the start of the power pulse and then continued (i.e. "restarted") with 6 cracks. The outcomes of this simple study are shown in Figure 4, where the cladding axial deformation is plotted for all cases.

To the authors' knowledge, the limitations of TRANSURANUS code are common to other 1.5D fuel performance codes, and a realistic and accurate modelling of the fuel cracking behavior in all situations of interest is still an open, challenging issue, which deserves substantial R&D efforts. Perhaps, some progress may be expected from applying 2D or 3D finite element modelling with a mechanistic description of the phenomena involved.
Work is in progress at Institute for Transuranium Elements (ITU) to improved TRANSURANUS capabilities to model the behavior of cracked fuel.

As mentioned above, the sensitivity analysis consisted in calculating Spearman's rank correlation coefficients for each specified outlet variable (evaluated at each relevant time reported in Table III, and at maxima, for a total of 6 values) with respect to each specified inlet parameter. Six 19 x 9 tables are thus obtained. Table IV is an upper envelope of those six tables, and summarizes the outcomes of the sensitivity analysis. Coefficients values between 0.25 and 0.5 are highlighted in yellow and those higher than 0.5 are highlighted in green. This allows pointing out the most important sensitivities.
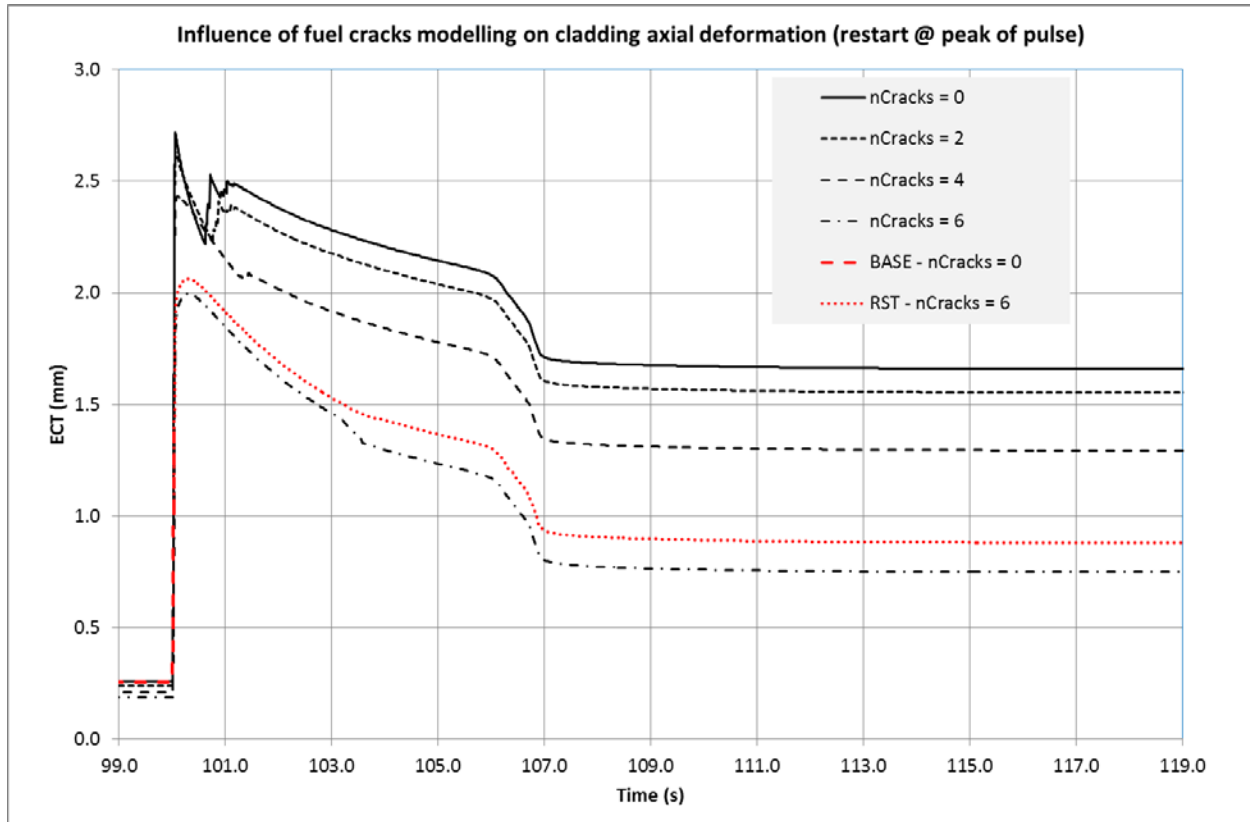
Figure 4. Effect of number of fuel cracks on mechanical behavior.

Table IV. Spearman's rank correlation coefficients (global table).

INPUT PARAMETERS	OUTPUT PARAMETERS								
	DHR	TFC	TFO	TCO	ECTH	ECT	EFT1	SCH	RFO
Cladding outside diameter	8.70E-02	6.15E-02	9.27E-02	7.84E-02	6.64E-02	7.44E-02	9.59E-02	4.40E-01	1.01E-01
Cladding inside diameter	3.65E-02	1.18E-01	1.18E-01	1.18E-01	1.93E-02	2.40E-02	6.11E-02	5.57E-01	9.98E-01
Fuel theoretical density	8.51E-02	8.72E-02	6.87E-02	6.85E-02	8.52E-02	5.24E-02	6.23E-02	9.63E-02	8.46E-02
Fuel porosity	9.50E-02	1.07E-01	7.75E-02	1.20E-01	1.02E-01	5.44E-02	1.61E-01	9.41E-02	1.04E-01
Cladding roughness	1.66E-01	1.35E-01	3.85E-01	1.37E-01	9.36E-02	7.32E-02	1.41E-01	1.03E-01	3.98E-02
Fuel roughness	1.34E-01	1.56E-01	2.69E-01	9.74E-02	1.20E-01	1.07E-01	1.75E-01	1.04E-01	1.24E-01
Filling gas pressure	1.63E-01	1.68E-01	1.57E-01	1.56E-01	1.98E-01	2.10E-01	2.10E-01	4.58E-01	2.05E-01
Coolant pressure	1.37E-01	1.39E-01	1.32E-01	1.21E-01	1.85E-01	1.81E-01	1.81E-01	4.84E-01	2.40E-01
Coolant inlet temperature	3.59E-01	1.00E+00	1.00E+00	1.00E+00	1.37E-01	1.57E-01	1.51E-01	1.26E-01	1.23E-01
Coolant velocity	4.37E-02	7.55E-02	7.54E-02	7.53E-02	4.04E-02	4.36E-02	4.87E-02	7.03E-02	2.34E-02
Injected energy in the rod	9.67E-01	9.29E-01	9.07E-01	8.44E-01	7.97E-01	6.96E-01	8.89E-01	2.55E-01	6.13E-01
Full mid height width	6.88E-01	6.64E-01	4.60E-01	5.43E-01	6.30E-01	6.36E-01	6.34E-01	4.41E-01	6.39E-01
Fuel thermal conductivity	1.65E-01	1.00E-01	1.24E-01	1.00E-01	4.56E-02	4.95E-02	4.94E-02	1.93E-01	3.52E-02
Clad thermal conductivity	6.04E-02	8.96E-02	8.97E-02	8.95E-02	1.06E-01	9.22E-02	7.64E-02	1.31E-01	5.81E-02
Fuel thermal expansion	1.38E-01	1.37E-01	1.48E-01	1.30E-01	7.23E-01	7.15E-01	6.25E-01	8.18E-01	5.12E-01
Clad thermal expansion	1.47E-01	1.45E-01	1.35E-01	1.15E-01	5.36E-01	8.63E-01	7.40E-01	6.54E-01	2.12E-01
Clad Yield stress	9.47E-02	1.13E-01	1.13E-01	1.13E-01	2.03E-01	2.68E-01	1.81E-01	9.97E-01	7.41E-02
Fuel enthalpy	9.40E-01	2.44E-01	1.45E-01	7.31E-02	2.09E-01	1.93E-01	2.14E-01	1.23E-01	1.90E-01
Clad to coolant heat tr.	1.99E-01	6.93E-02	6.32E-01	7.13E-01	1.67E-01	1.60E-01	1.57E-01	1.73E-01	1.30E-01

5. CONCLUSIONS

An in-house software tool, termed StaRT, was developed and utilized for performing a Monte Carlo RELAP5/TRANSURANUS coupled calculation of an idealized RIA scenario and providing uncertainty quantification and sensitivity analysis. This work was performed in the framework of the "RIA fuel performance benchmark" organized by the OECD WGFS.

The StaRT tool, although specifically implemented for the benchmark purposes, can in principle easily be adapted for more general use. The development work was preparatory to other R&D activities, in progress at NINE, related to code uncertainty quantification methods and multi-physics code applications. The benchmark results will soon be published by the WGFS and are not discussed in this paper.

The exercise, although based on a relatively simple problem, presents quite challenging modelling issues, particularly as regards the TH evolution and the effects of fuel cracking on both fuel and cladding stress and strain status throughout the transient, as shown by the presented results. The cracking behavior is further complicated when power changes are fast, such as in RIAs. Moreover, the initially fresh (and thus un-cracked) fuel assumed by the exercise is expected to undergo an immediate cracking process which is hard to characterize and model. Most fuel performance codes, including TRANSURANUS, can deal with such modeling issues only in a limited way, and further development and validation efforts are necessary, possibly involving multi-dimensional modelling.

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