McSAFE

High-Performance Monte Carlo Methods for SAFEty Demonstration-From Proof of Concept to realistic Safety Analysis and Industry Applications

Research and Innovation actions

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D6.3: Third Synthesis Report

Summary

In this report the progress and achievements obtained during the period September 2019 till September 2020 of the McSAFE project are presented for interested parties and possible users of the advanced computer codes and methods for accurate nuclear reactor calculations that will be available after completion of the project.
The Monte Carlo codes used in the project are Serpent2, TRIPOLI-4®, MONK® and dynMCNP6. As most of the development or improvement of the Monte Carlo methods needed for full-core static and transient calculation, possibly with burnup, and its coupling with thermal-hydraulics and thermo-mechanics was developed in the pervious periods of the project, the emphasis of the project work in the last year was devoted to validation of the methods.
Validation examples are shown for a mini-core ,a full-scale PWR, a full-scale VVER and the small SPERT IIIE reactor with a fast transient. All validation examples include coupling with the SubChanFlow thermal-hydraulics code. In various cases also coupling with the thermo-mechanics code TRANSURANUS is applied. Moreover, depletion calculations for a full-scale reacttemperature coefor are validated.
It is concluded the the project was successful in almost all planned activities according to the original Description of Work and delivers highly sophisticated, validated Monte Carlo codes for static and dynamic calculation, with advanced depletion option, and with and coupling to thermal-hydraulics and thermo-mechanics codes. It can be stated that these code combinations set a new mark in high-fidelity integrated nuclear reactor calculations.

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Distribution to the partners will be through the project SharePoint.

Content

1. Introduction

The overall objective of the McSAFE project [1] is to move the Monte Carlo based stand-alone and coupled solution methodologies to become valuable and widespread numerical tools for realistic core design, safety analysis and industry-like applications of LWRs of generation II and III. As Monte Carlo codes are very flexible with respect to reactor geometry and composition, the results of the project will also be useful for future types of nuclear reactors as well as to research reactors with complicated geometries and unusual contructions for experimental research applications. Main targets in the development are advanced depletion, optimal coupling of Monte Carlo codes to thermal-hydraulic and thermo-mechanical solvers, time-dependent Monte Carlo and methods for massively parallel simulations.

On one hand, the envisaged developments will permit to predict important core safety parameters with less conservatism than current state-of-the-art methods. On the other hand, they will make possible the increase in performance and operational flexibility of nuclear reactors.

We foster the dissemination of knowledge gained in the project by experienced researchers to become available to any interested party and possible future users of the codes and code systems under development. To that end several actions are executed, like a tailored training course for interested persons, digital newsletters and synthesis reports. The first newsletter was sent out in August 2018. A second newsletter was issued in August 2019. A third newsletter will be issued directly after the project is ended.

Within this scope of dissemination of results, the synthesis reports are issued to inform interested parties about the goals and progress made in the McSAFE project. The first synthesis report covered the first one and a half year of execution of the McSAFE project and was issued in February 2019. The second synthesis report covered the next 6 months of the project. The current report is the third and last synthesis report and covers the last 12 months of the project.

Moreover, to boost the exploitation of project results, an exploitation plan was issued as well as a detailed dissemination and communication plan, in which potential users of the McSAFE tools and methods were identified with the help of all project partners.

An overview of the McSAFE project is represented at the international FISA conference in Pitesti, Romania and at the Physor conference in Cambridge, UK, March/April 2020. Various presentations about specific parts of the research were given at several international conferences like the ICONE conference in Tsukuba, Japan, May 2019, the ICAPP conference, Juan-les-Pins, France, May 2019 and the Physor conference in Cambridge, UK, March/April 2020. Many papers are published or submitted to international scientific journals like Annals of Nuclear Energy.

2. The McSAFE Project

Monte Carlo methods are nowadays in wide spread use for nuclear reactor calculations. Although their capabilities have increased considerably over the last decades, supported by the increase in computer power, calculation of detailed power distributions throughout the core of a full-size reactor with sufficient statistical accuracy in acceptable computing time is still questionable.

Moreover, for reactor operation evaluation the actual temperature distribution in the reactor core must be taken into account. Hence, coupling of the Monte Carlo calculation with a thermal-hydraulic calculation is necessary, which must normally be executed in an iterative way. Also the thermo-

mechanical behaviour of the reactor core must be taken into account. Hence, coupling of the Monte Carlo code with a thermo-mechanical code has become a prerequisite for reactor calculations.

Another challenging task for Monte Carlo is a proper depletion calculation. Most general-purpose codes devoted to reactor physics have an option for depletion calculations, but they take long calculation times and their stability can often be questioned.

For safety analysis not only the static properties of the reactor core are important, but also the dynamic behaviour of the core. This requires the extension of the Monte Carlo code with time dependence. For prompt neutrons this time dependence is often included in the original codes, but for transient reactor calculations delayed neutrons and their precursors are of utmost importance and require a separate treatment in the Monte Carlo code. Transient calculations also require adequate modelling of control rod movements and, for instance, boron dilution.

This gives a sketch of the main lines of the McSafe project [1]: to develop Monte Carlo codes suitable for Monte Carlo calculations coupled with thermal-hydraulics and thermo-mechanics for a full-size reactor core, including depletion (burnup) and time-dependence for reactor transients. Coupled codes can be implemented in the NURESIM computer platform [2,3], which is based on the Salomé platform [4].

Participants in the McSAFE project are:

Karlsruhe Institute of Technology (KIT, coordinator; Germany)

Delft Nuclear Consultancy (DNC; The Netherlands)

Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA; France)

UJV Rez, a.s. (UJV;Czech Republic)

Helmholtz-Zentrum Dresden-Rossendorf (HZDR; Germany)

Jacobs (Jacobs; United Kingdom)

Technical Research Centre of Finland (VTT, Finland)

Royal Institute of Technology (KTH; Sweden)

Joint Research Centre (JRC; EU)

E.ON Kernkraft GmbH (EKK; Germany)

CEZ a. s. Nuclear Power Plants (CEZ; Czech Republic)

Electricité de France (EdF; France)

Each partner brings in its typical experience to one or more of the subjects under development in the McSAFE project. This can be a general-purpose Monte Carlo reactor code, a thermo-hydraulics or thermo-mechanics code, experience in coupling codes or in depletion or time-dependent calculations or providing reactor plant data for validation of the developed code combinations.

In the McSAFE project 4 different Monte Carlo codes are considered, 3 of them being developed in Europe: Serpent2 (VTT), TRIPOLI-4® (CEA) and MONK® (Jacobs). The US Monte Carlo code MCNP6 (LANL) is extended and tailored for the project by DNC. The thermo-hydraulics code used in the project is SubChanFlow (SCF; KIT). The thermo-mechanics code used in the project is TransUranus (TU, JRC).
The McSAFE projects benefits from the achievements of the former EU HPMC project. Its goals are in line with the priority topics of NUGENIA and the SNETP platform.

A broad overview oft he project research subjects and achievements were presented in a training course on June 22-24, 2020, for interested people, which was organised as a video conference because oft he restrictions due to the COVID19 pandemic. Twenty four participants from twelve

different countries and three continents attended the course, these being representatives of universities, research centres, industries and regulators.
During the course eighteen lectures were given by experts from several McSAFE partner organisations (KIT, VTT, CEA, JRC, DNC and UJV). During the presentations a comprehensive overview of the McSAFE achievements has been provided through a mixture of theoretical lectures and demonstrations on the applications for base cases of the different coupling tools developed within the project. A report with a summary of the presentations of the training course was completed as a deliverable of the project.

3. Progress in Monte Carlo methods for depletion calculations

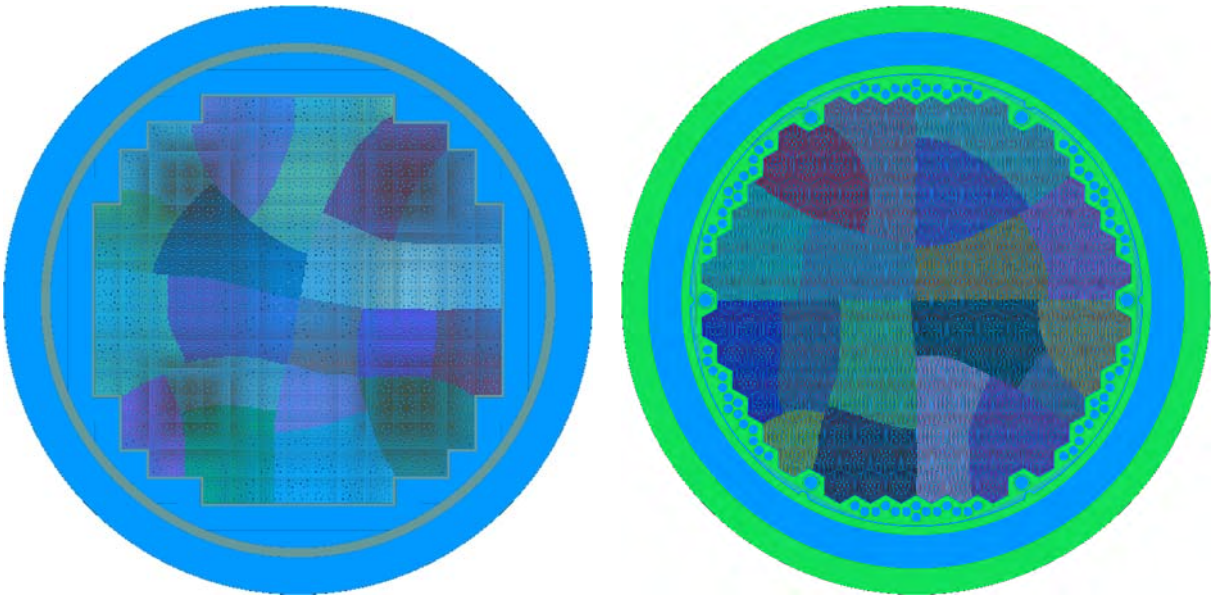
In the McSAFE project the Monte Carlo method is the corner stone for neutron transport. Although each of the Monte Carlo codes used in the project has been developed for a long time and has a history of continuous extentions and improvements, several items are identified for further improvement to achieve the efficiency needed for detailed full-core calculations. Therefore, various participants worked on smaller and larger improvements, which were successfully implemented in the Monte Carlo codes during the project. Some achievements from the last year,especially with regard to depletion calculations, are detailed here.

3.1 Domain decomposition for depletion calculations

Full-core pin-by-pin depletion problems in Serpent 2 can take several TB of RAM memory, mainly in order to store the compositions and additional data for burnable materials. This exceeds the memory available in each single node for any High Performance Computing (HPC) architecture, and therefore creates a bottleneck that needs to be tackled to even start running such cases. To solve this issue, a Collision-based Domain Decomposition (CDD) scheme was implemented in Serpent 2 [5]. The idea of the method is to define domains containing only a subset of the burnable materials, while all other model data, such as geometry, non-burnable materials and spatial tallies, is replicated in all domains. Doing this, the memory footprint of the burnup calculation is split across nodes (MPI tasks), and a problem that does not fit in a single node can be solved by adding computing nodes until the memory for each MPI task fits in each node. The tracking algorithm is modified to account for neutrons flying across domains when they have collisions in non-local materials, but the method does not rely on any numerical or physical approximations and hence the results are equivalent to the traditional Monte Carlo approach, within their statistical uncertainty.

As an example, Fig. 1 shows the material decomposition for the PWR and VVER validation cases presented in the next section. Each domain is comprised of the fuel materials of a given colour and all other information about the system. The decomposition is performed using a graph-partitioning method, in both cases for simulations using 64 domains.

Fig. 1. Material decomposition for the PWR validation case in the next section.

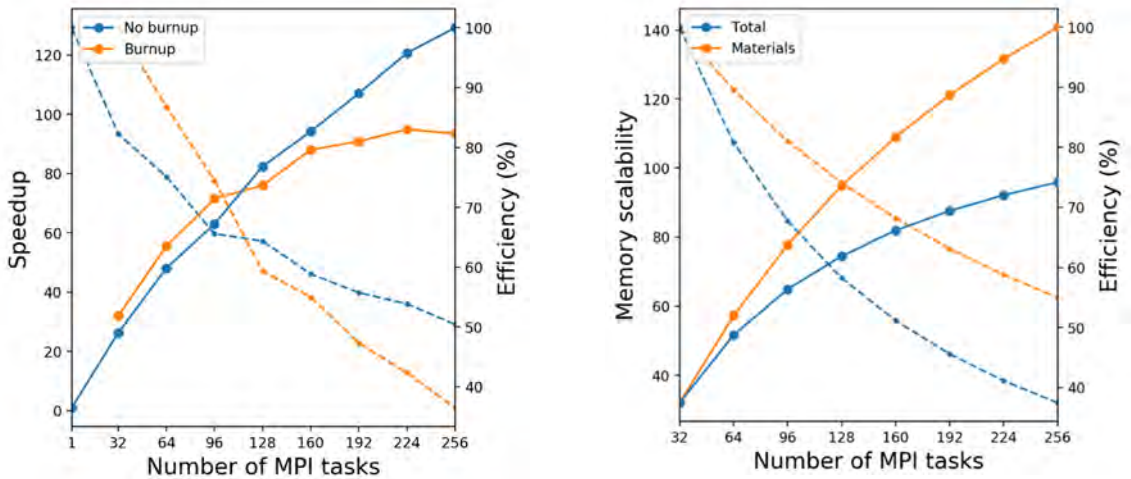


a) PWR domain decomposition – xy cut

b) VVER domain decomposition – xy cut

These scalability tests were performed in the ForHLR II computer system running relatively short simulations, of the order of a few hours of wall clock time. The performance is calculated as a function of the number of nodes, and in all cases all 20 available cores per node are used with OpenMP multithreading, meaning that the tests go up to a total of 5,120 cores, which is quite massive for these types of codes. For these tests, the availability of such high number of nodes was exceptionally useful.

Fig. 2. Speedup and memory scalability for the CDD scheme.



a) CPU speedup

a) RAM memory scalability

3.2 Tally decomposition

The reaction rate tallies required by the depletion solver during a whole core burnup calculation can have a significant memory footprint; replicating the tally array across multiple parallel processes can make the problem intractable. Instead, distributing the tallies can reduce the total memory requirement, allowing cases with large numbers of depleteable materials to be handled efficiently.

Here we are not considering spatial or material domain composition, so each process will simulate reactions in materials for which it is not responsible for tallying. Therefore each process needs to buffer such events and periodically communicate them to the processes responsible for tallying them. There is a memory and run-time cost for storing these buffers and communicating them to other processes, but with an optimal algorithm it is found to be possible to achieve a net reduction in memory footprint with minimal performance impact.

Such a scheme has been trialled using a simple Monte Carlo code to represent the salient features of a Monte Carlo depletion calculation, designed specifically for the task. The results demonstrate that tally decomposition works to good effect in two important scenarios. The first is to allow all CPU cores on a compute node to be used in cases where this would not be possible without tally decomposition. The second is to allow cases which do not fit within the memory on a single node to be distributed across multiple nodes. The run time penalty in all cases considered is acceptable, and is negligible compared to typical runtimes for Monte Carlo whole core depletion calculations.

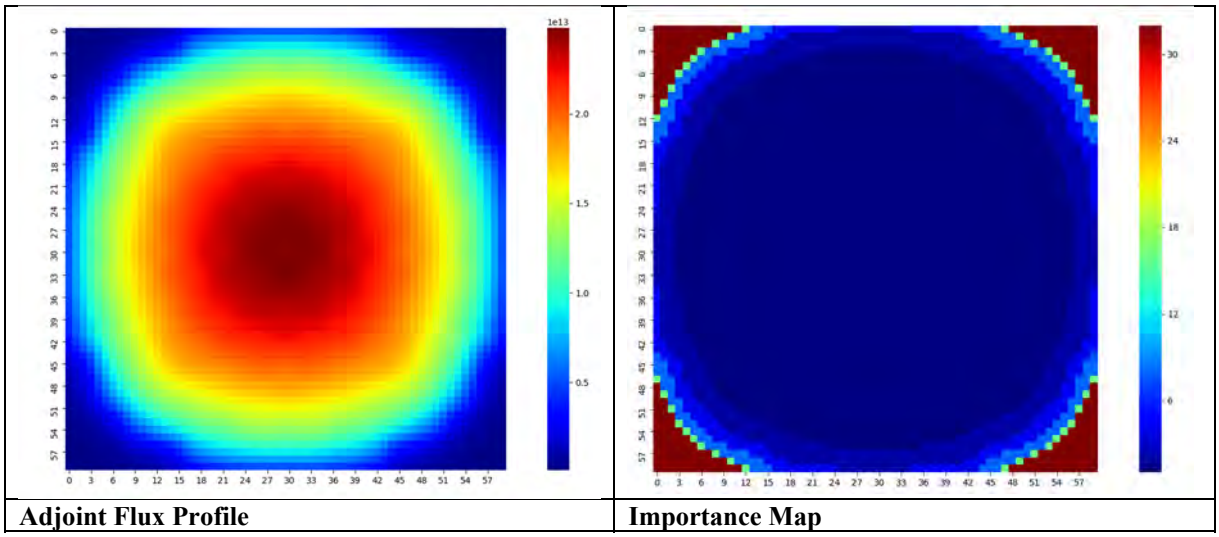
3.3 Variance reduction for depletion calcuations

In a standard reactor physics Monte Carlo calculation the neutrons are targeted preferentially at the more reactive central regions of the core. This is the ideal strategy for converging the neutron multiplication factor for a reactor. However, the statistics will be better towards the centre of the core and worse towards the outer edges of the core. Hence the flux and consequently the composition of the outer fuel pins will be determined less accurately at the edge of the core. This is not ideal for a depletion calculation whose aim is to determine the composition of all fuel pins discharged from the reactor.

An importance map has been introduced to flatten the variance across the core. Monte Carlo criticality codes use an iterative scheme that targets neutrons towards the more reactive regions of the core. It is known that the adjoint flux can be used as an importance map, that will target neutrons towards the more reactive regions. Therefore the inverse of the adjoint flux can be used to undo the tendency of the iterative scheme to target more reactive regions of the core and thus flatten the variance profile across the core. Such a scheme has been prototyped using the MONK® Monte Carlo criticality and reactor physics code.

For the Nakagawa and Mori PWR whole core benchmark the calculated adjoint flux and the derived importance map are shown in the Figs. 2 and 3.

Fig. 3. Adjoint flux and importance map



Adjoint Flux Profile | **Importance Map**

If the target is to determine the composition of all fuel pins to an accuracy of within 5% the improvement in performance when using an importance map is shown in the table below.

Table I. Number of Scoring Stages to achieve SD < 5% on all fuel pins

	Number of scoring stages required	CPU time (days) (inc. settling)
Reference	190	2.90
Importance Map	81	1.90
Change	-57%	-34%

For this particular application it is seen that the use of the importance map more that halves the number of scoring stages required to achieve the target standard deviation on the composition in all of the fuel pins and reduces the required CPU time by more than one third.

3.4 Multi-physics interface

A new multi-physics interface has been developed for TRIPOLI-4®. Preliminary details have been provided in the previous Synthesis Report. The SALOME-based interface has been extensively tested for the TMI fuel assembly simulations in stationary regime [6] and for the mini-core benchmark in transient regime [7]. This new interface can now be controlled by a C++ supervisor, which allows performing efficient coupling with other simulation codes.

4. Progress in time-dependent Monte Carlo calculations

4.1 Variance reduction in time-dependent Monte Carlo

Time-dependent Monte Carlo transport simulations involve very different time scales for neutrons and precursors, which demand distinct variance reduction techniques with respect to stationary simulations. Additionally, the delayed neutron fraction (stemming from precursor decay) is very small, which might lead to serious under-prediction biases. In order to cope with these issues, we have implemented several strategies in TRIPOLI-4®, including forced precursor decay, branchless collisions, importance sampling of the neutron and precursor populations, and several population control techniques (Russian Roulette and splitting and “combing”). These strategies have been extensively investigated in the framework of a benchmark configuration based on a TMI fuel assembly: these findings have been published in [8].

During the final year of the project, we have investigated the feasibility of *zero-variance schemes* for time-dependent transport, including the contribution of precursors. Such schemes, based on a generalisation of the well-known CADIS (Consistent Adjoint-Driven Importance Sampling) strategy for stationary (i.e., time-independent) simulations, have been developed by a suitable extension of the moment equations originally proposed by Lux and Koblinger. The basic idea is to use the (exact or approximate) solutions of the adjoint time-dependent Boltzmann equation, coupled to the (adjoint) equation for the evolution of the delayed neutron precursors, in order to derive a modified source and modified flight and collision kernels to “optimally” guide the neutron towards the detector. When the adjoint solutions are known exactly, such schemes can in principle yield Monte Carlo estimates with zero variance. We have also provided a proof of principle of such time-dependent CADIS approach for a simplified transport problem: numerical findings have shown that this strategy has

the potential to unlock enormous gains for the figure of merit of the kinetic Monte Carlo calculations, which are notoriously difficult. A preliminary version of this work has appeared in the Physor 2020 proceedings [9] and a full detailed treatment has been published in a journal paper [10].

5.2 Improvement of parallelisation for time dependence

The performance of OpenMP parallelisation in dynamic problems can deteriorate due to variations in fission chain lengths simulated by the different OpenMP threads:

To mitigate this problem, two approaches for OpenMP load balancing were investigated:

1. A thread-common simulation queue, where the simulation queue of secondary particles is either fully or partially shared by the different OpenMP threads.

2. A generation based simulation approach, where the simulation queue is re-distributed equally across the OpenMP threads after the simulation of each generation of particles.

Both approaches led to significant improvements in the OpenMP scalability of the simulations with the thread-common simulation queue generally having a slightly better performance than the generation based approach

Table II OMP scalability of transient simulation with branchless Monte Carlo as a function of primary source size and number of OpenMP threads. Averaged over 5 simulations. No OpenMP load balancing.

Primary source size (particles)	*Number of OpenMP threads*			
	1	*4*	*16*	*28*
2000	*100 %*	*100 %*	*37 %*	*28 %*
8000	*100 %*	*123 %*	*74 %*	*62 %*
32000	*100 %*	*102 %*	*80 %*	*64 %*

5. Validation of computer codes

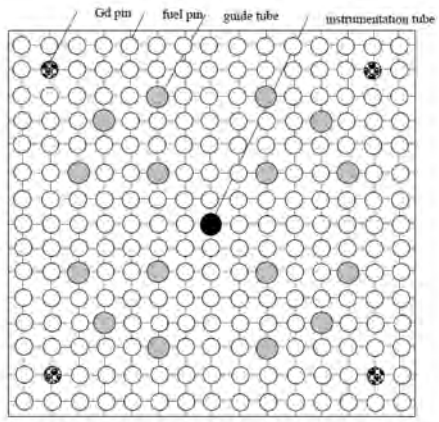
The validation of the tools developed in the project is partly conducted against operational data from power plants. The actual operation of power plants differs somewhat from classical use-cases of Monte Carlo reactor physics codes including power and control rod maneuvering, which need to be accurately modelled by the reactor physics code if reasonable agreement between simulations and measurements is expected.

While Serpent previously offered a capability to modify reactor power during a single depletion calculation, each depletion calculation was executed using a static geometry. Recently, we extended Serpent to apply any variations described by branch definitions (http://serpent.vtt.fi/mediawiki/index.php/Input_syntax_manual#branch_.28branch_definition.29) during depletion calculations. The main advantage for this subproject lies in the ability to define control rod movements, but as the capability is generic other uses, such as inserting detectors to instrumentation tubes, etc., can be also foreseen.

5.1 Validation for a mini-core

The coupling of the three codes SERPENT, SubChanFlow and TRANSURANUS under the European reactor simulation platform NURESIM using the ICoCo interface was accomplished successfully. Test cases with single pins as well as single fuel assemblies in rectangular and hexagonal geometry were used for testing the coupling. The next step of the testing was the benchmarking of the coupling and the comparison to the coupling of the three codes using the multi-physics interface of the Monte Carlo code SERPENT. For that purpose, a benchmark was defined for the quadratic and for the hexagonal geometry options. Both cases consider mini-cores at hot full power at equilibrium Xenon concentration in order to test the interaction of the three codes in the two different environments (ICoCo and direct interface). Here some results of the PWR mini-core are presented. Fig. 4 shows the layout of one fuel assembly derived from a realistic assembly description of the NPP TMI-1 and the mini-core cross section with rodded (R) and unrodded (U) fuel assemblies. Fig. 5 shows the SERPENT model which replicates the mentioned mini-core. Steady-state calculations using both above mentioned approaches have been conducted. Fig. 6 shows the corresponding coolant outlet temperature for both approaches and Fig. 7 the averaged fuel pin temperatures in the central fuel assembly. The comparison between the two coupling options shows a very good agreement both at fuel assembly and local (pin) level.

Fig. 4: Layout of the fuel assembly and the mini-core for the quadratic case



Reflector	Reflector	Reflector	Reflector	Reflector
Reflector	U	U	U	Reflector
Reflector	U	R	U	Reflector
Reflector	U	U	U	Reflector
Reflector	Reflector	Reflector	Reflector	Reflector

Fig. 5: Cross section of the Serpent PWR mini-core model

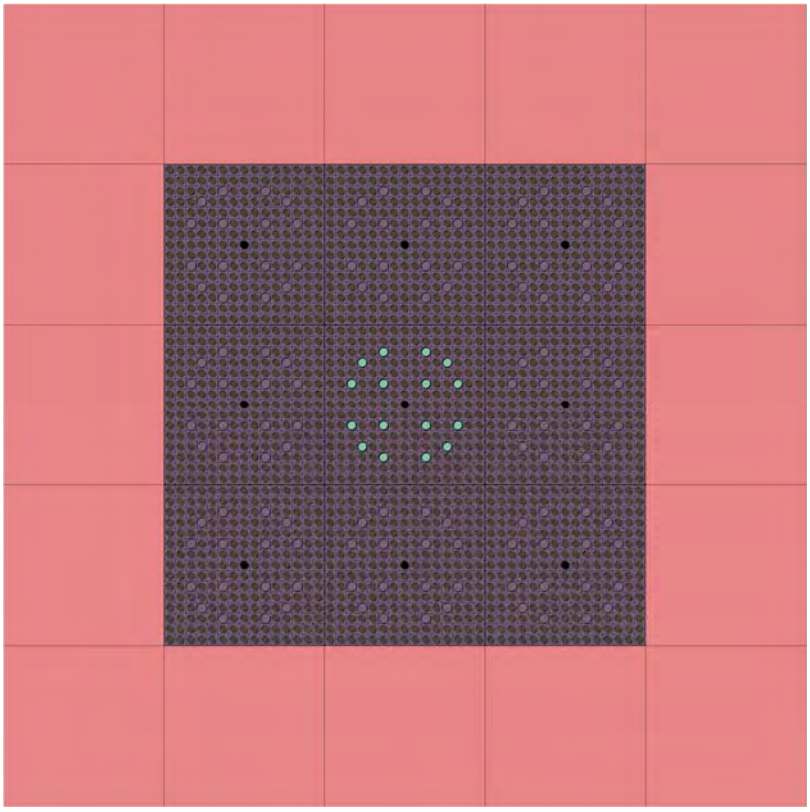


Fig. 6: Channel outlet temperature in the case of ICoCo (a) and Internal (b) couplings

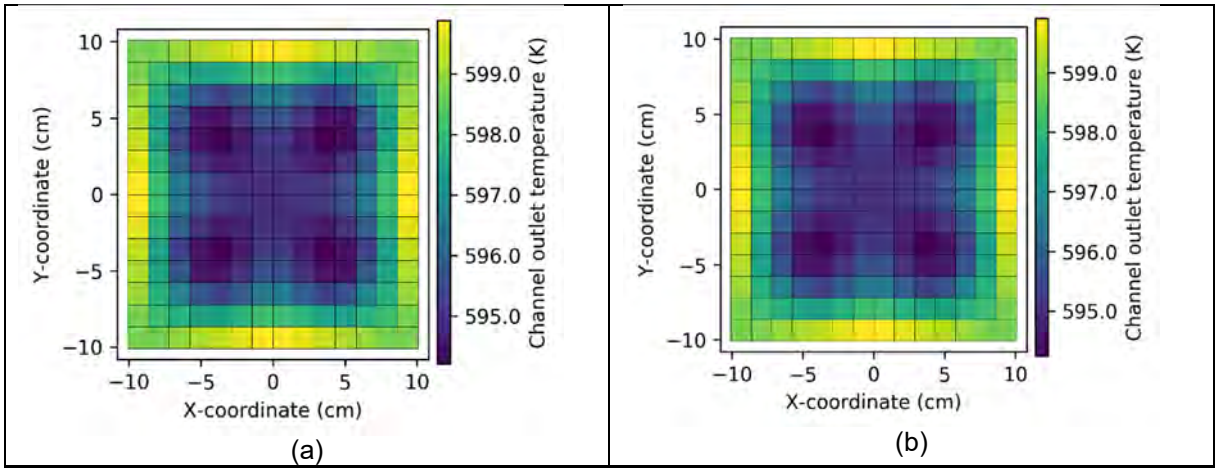
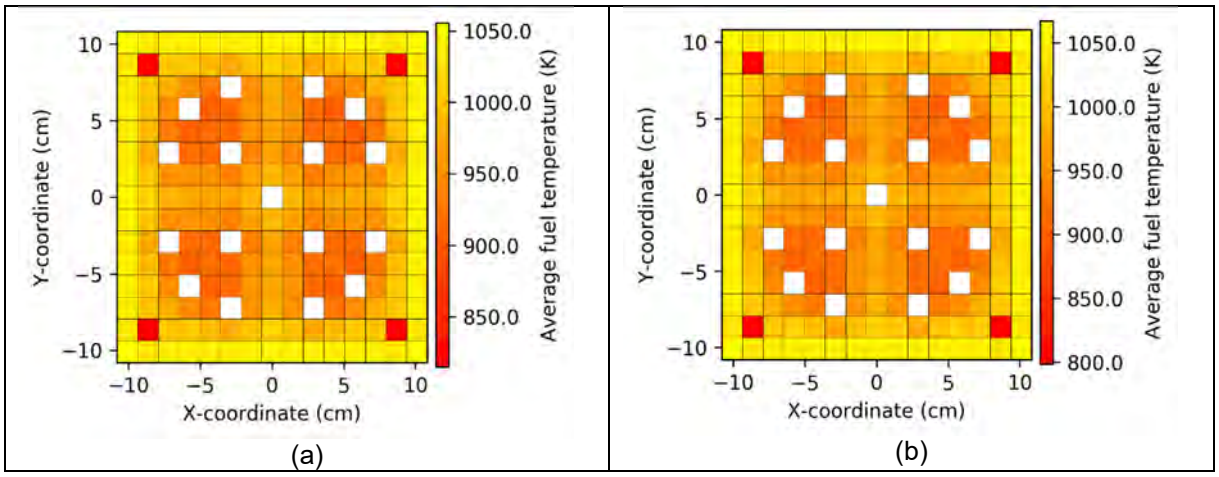


Fig. 7: Average pin fuel temperatures for the central FA in the case of ICoCo (a) and Internal (b) couplings



The final step before entering the full-core calculations has been the testing of the coupled depletion capabilities, including the newly implemented CDD scheme, which solves the memory bottleneck for the full-core calculations. The test proceeded on a VVER-1000 mini-core case composed from seven VVER-1000 fuel assemblies surrounded by a water reflector with black boundary condition. Two ICoCo coupling schemes were tested: SSS2-SCF-TU and SSS2-SCF. Fig. 8 shows the calculation geometry and Fig. 9 the evolution of the multiplication factor with burnup: at the beginning the criticality search option in Serpent maintains critical state by adjusting boron concentration. When all the reactivity stored in boron is used, the core becomes subcritical.

Fig. 8. Core layout of the VVER-1000 mini-core

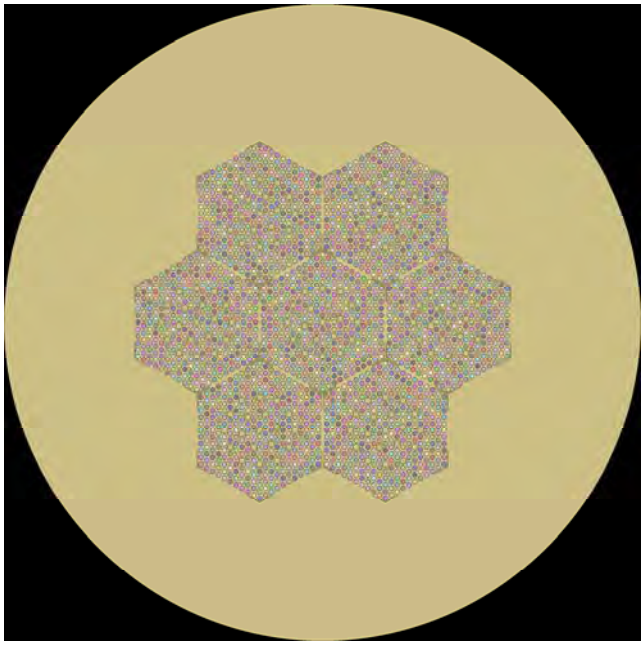
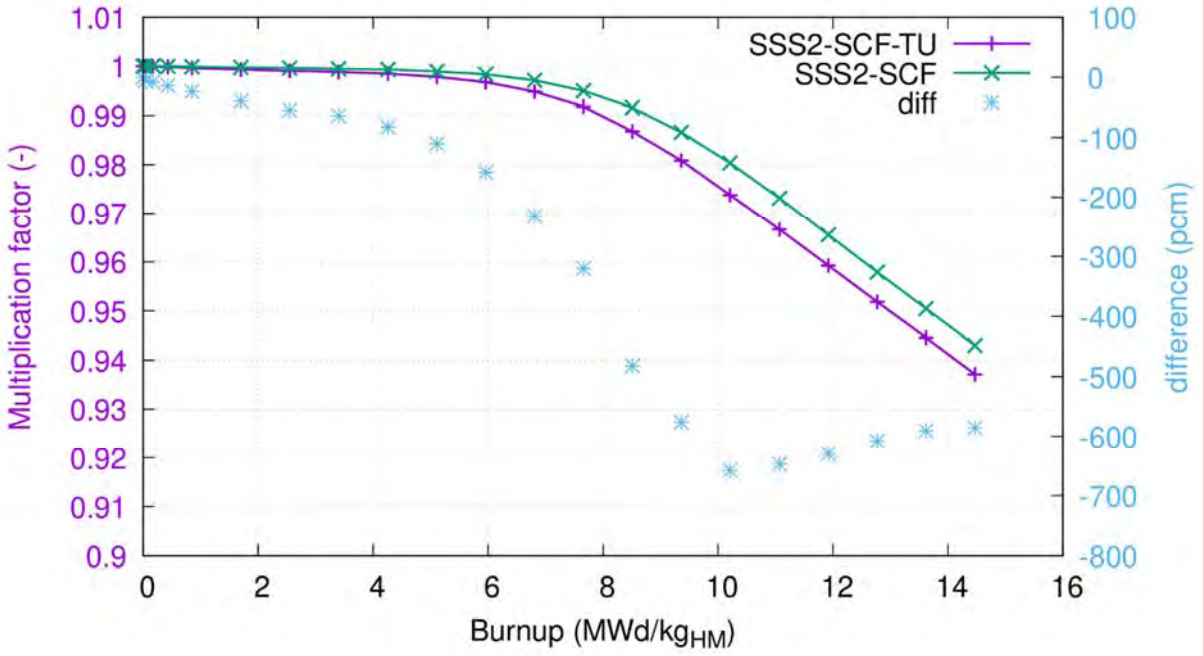


Fig. 9. Evolution of multiplication factor with burnup.

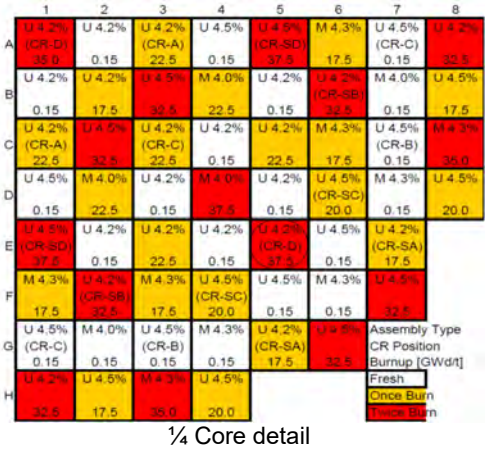


6.2 Validation for a full-scale PWR for transient capabilities

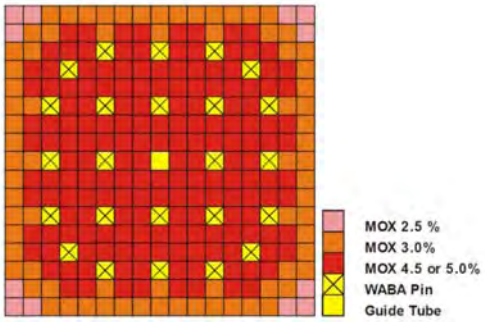
To evaluate the full-scope transient coupled capabilities of Serpent-SCF the well-known MOX/UO2 PWR transient OECD/NRC benchmark [11] was considered. This numerical exercise proposes a graded approach calculation for a full-scope PWR core with thermal-hydraulic (TH) coupling, aimed to develop a RIA-kind (Reactivity Insertion Accident) generated by a sudden control rod (CR) withdrawal.

This numerical benchmark proposes a series of calculations within a typical PWR core, loaded with mixed oxides fuel as presented in9. Full-core pin-by-pin coupled calculations are thus developed, both at HFP, HZP and for a RIA-kind scenario (driven by a sudden CR extraction of CR-D from Fig. 10, departing from a HZP condition), where the in-depth details can be directly obtained from 12.

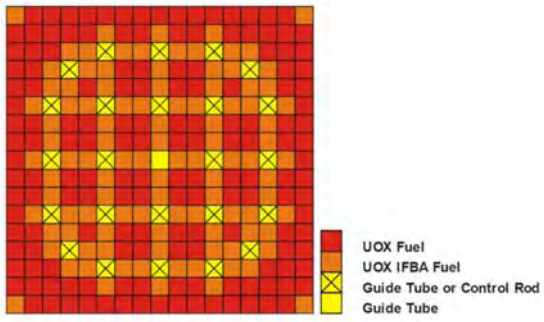
Fig. 10 MOX/UO2 PWR core 11



¼ Core detail



b) MOX FA



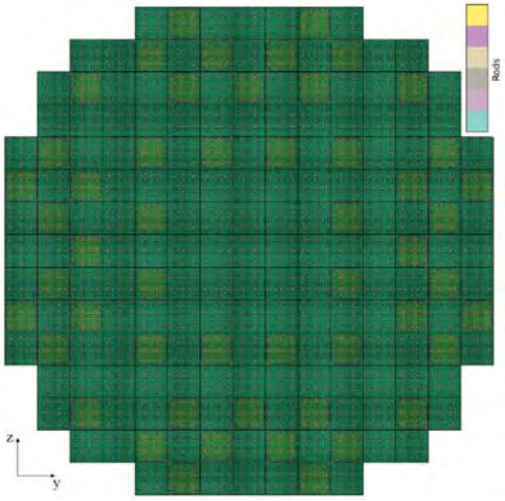
b)UO2 FA

The developed models, both for Serpent and SCF are presented in Fig. 11, where the control rod to execute the RIA scenario is identified.

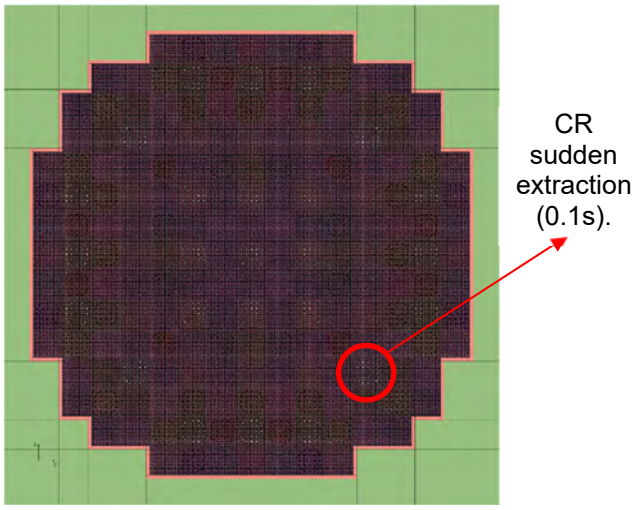
Main highlights are presented here for some parts of the analysis, where reported results within the benchmark are included for reference. It should be noted that this represents the first of kind coupled transient based in MC neutronics at a full-scope PWR with depleted compositions.

The results for HFP are presented in Fig. 12, where the consistency of power and temperature fields can be observed.

Fig. 11 MOX/UO2 PWR core Serpent and SCF models

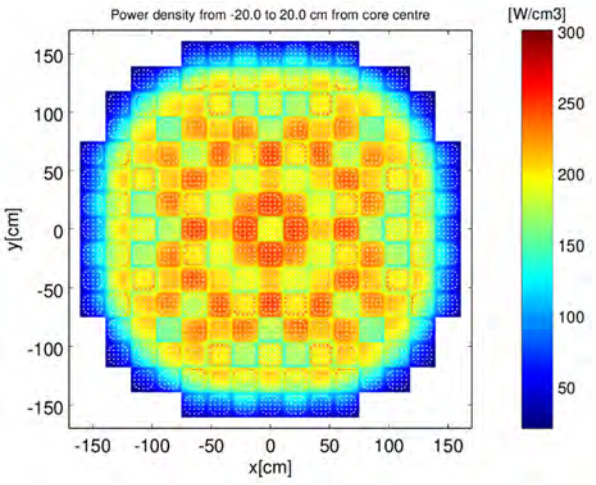


a) SCF model

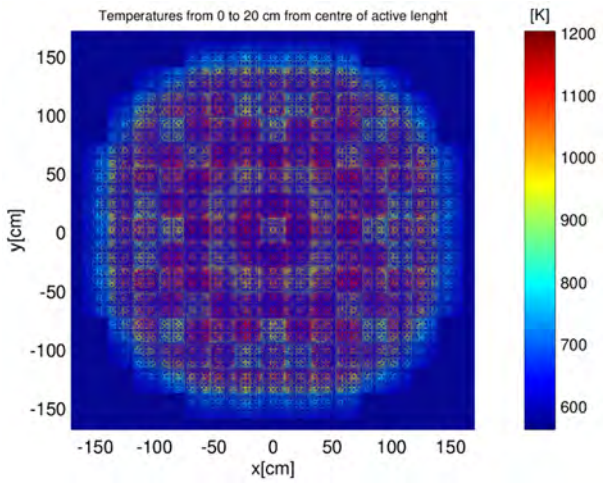


b) Serpent model – xy cut

Fig. 12 Serpent-SCF results for HFP case



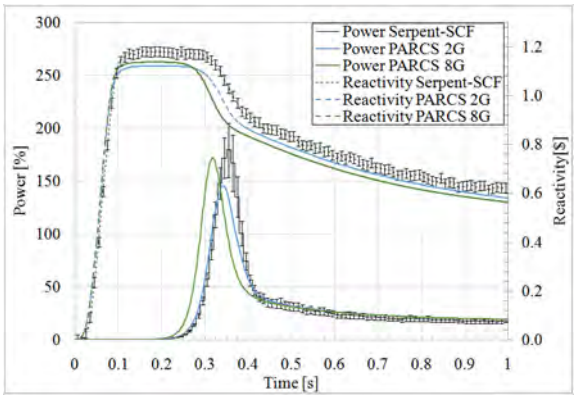
a) Power distribution at HFP



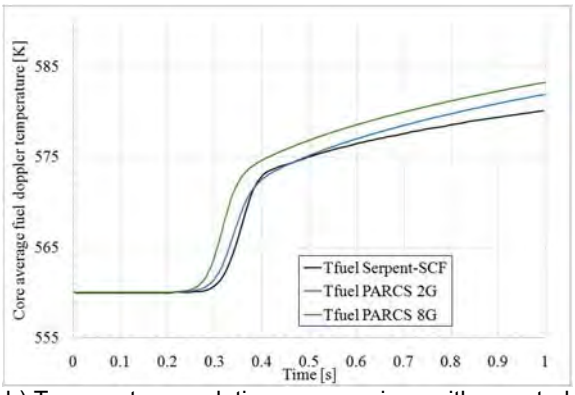
b) Temperature distribution at HFP

On top of that, the Fig. 13 represents the evolution of the main parameters for the RIA-kind transient compared with reported results, while Fig. 14 shows the high-fidelity features of the approach.

Fig. 13 Serpent-SCF results for the RIA case

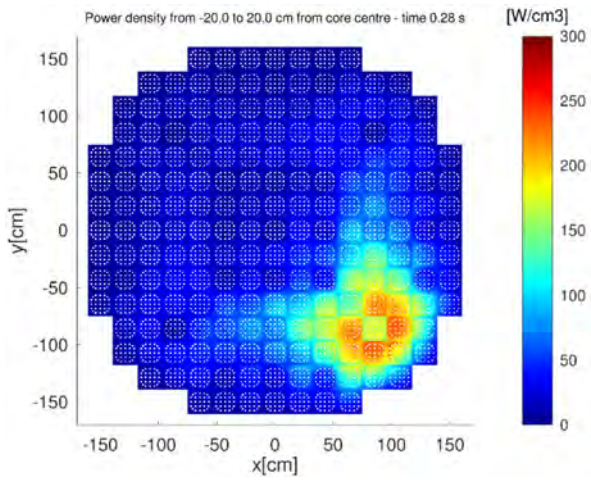


a) Power and reactivity evolution – comparison with reported results

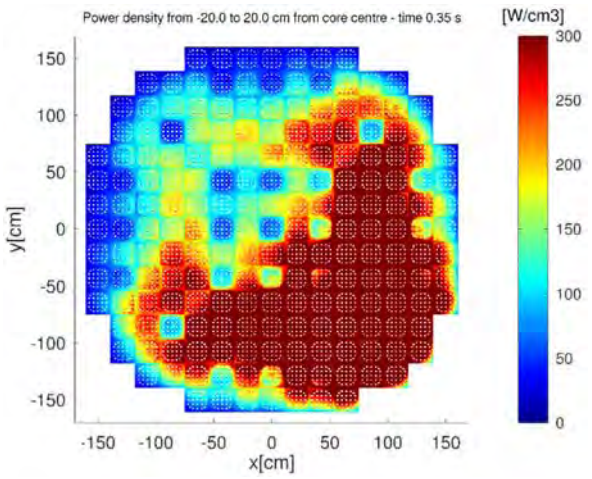


b) Temperature evolution – comparison with reported results

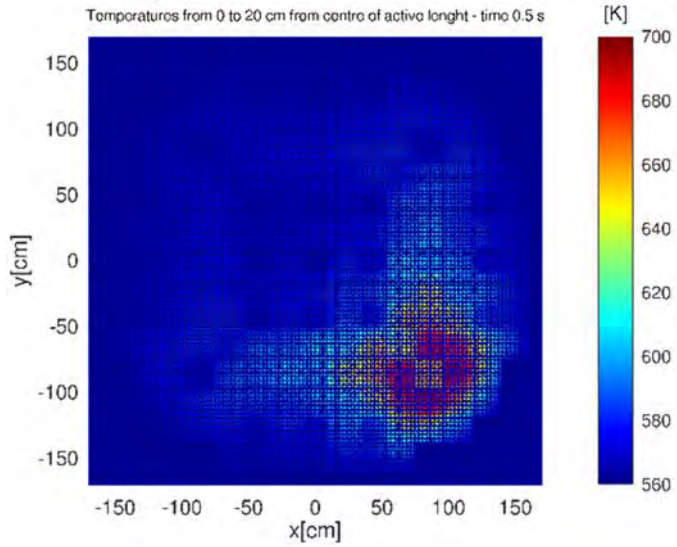
Fig. 14 Example of Serpent-SCF high-fidelity results for the RIA case



a) Power evolution for the RIA – xy cut 0.28 s



b) Power evolution for the RIA – 0.35 s



c) Temperature evolution – xy cut at 0.5s

After the verification of the coupling based on the mini-core calculations, measured data from nuclear power plants have been used for the validation of the coupled code system. For the validation of the quadratic geometry option, HZP (Hot Zero Power) data from the commissioning of a German PWR

have been used. The following data have been provided: critical boron concentration with all rods out, the isothermal moderator temperature coefficient and the control rod bank worth for different banks.

Based on the description of the first core configuration, input data sets for the different codes have been prepared. Fig. 15 shows the full core SERPENT model as horizontal cut and Fig. 16 the corresponding full core SubChanFlow model.

The comparison of obtained results in comparison to the plant measurements is summarised in Table. III. The moderator temperature coefficient (MTC) was calculated as a difference in reactivity between critical state (all control rods out, 1351 ppm boron concentration in coolant and 296.2˚C inlet coolant temperature) and the state with +8 K (304.2˚C) inlet coolant temperature divided by the temperature increment.

The worth of the control rod banks D1-4 was calculated as a difference in critical boron concentration between the all rods out state and the state with the corresponding bank fully inserted.

The obtained simulation results are in very good agreement with the measurements. The deviation in boron concentration is 18 ppm, which is 1.3 % of the measured value. The worth of the four control rod banks is predicted exactly. The biggest difference is observed in the moderator temperature coefficient, but it is considered satisfactory taking into account the MTC measurement uncertainty.

Table III: Comparison of simulation with measurement

	Experiment	*Serpent*	*Three-codes-coupling*
Crit. Boron, ppm	1351	1368	1369
MTC, pcm/K	11	7	7
D1 worth, ppm	30	31	31
D2 worth, ppm	38	39	39
D3 worth, ppm	38	39	39
D4 worth, ppm	30	31	31

To check the consistency of results, the HZP measurements were also calculated by stand-alone Serpent, assuming an equal temperature of all materials. As expected, results of stand-alone Serpent simulation practically coincide with results of the coupled simulation. That shows that any deviation of simulation from measurement is a result of modelling and measurement uncertainties, but not introduced by the coupling methodology.

Fig. 15: Horizontal cut of the SERPENT PWR model

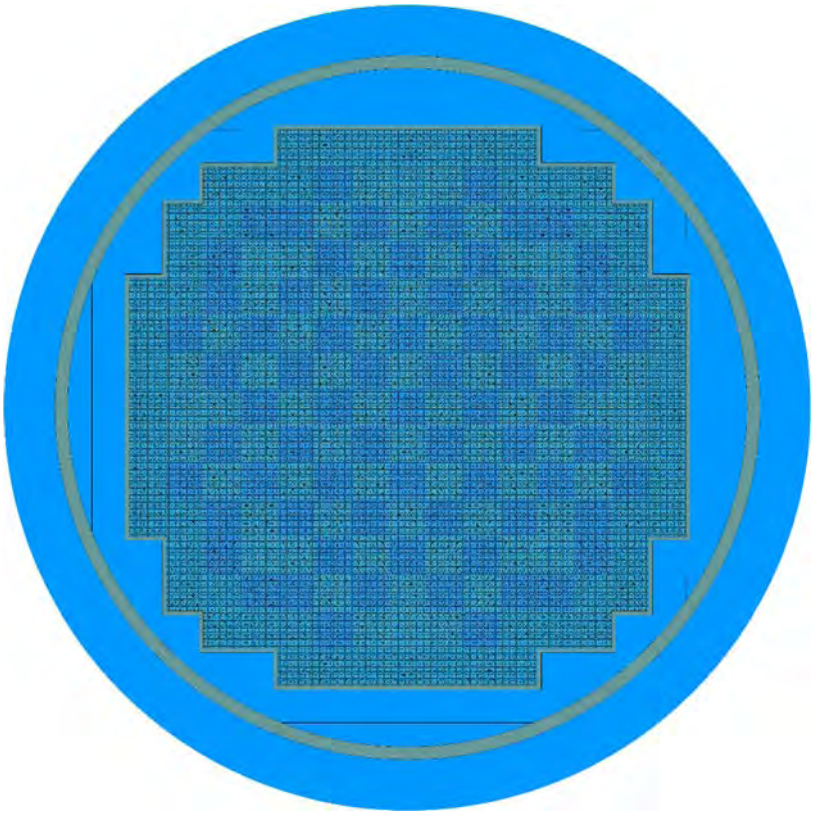
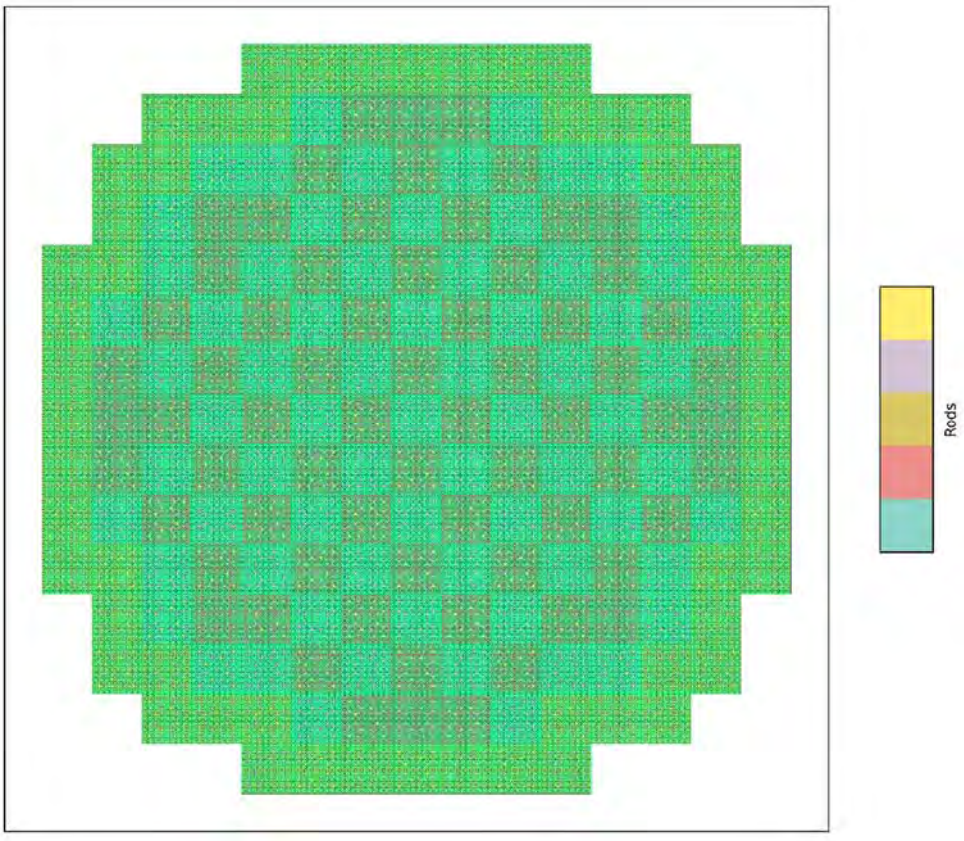


Fig. 16: SubChanFlow model of the PWR reactor core

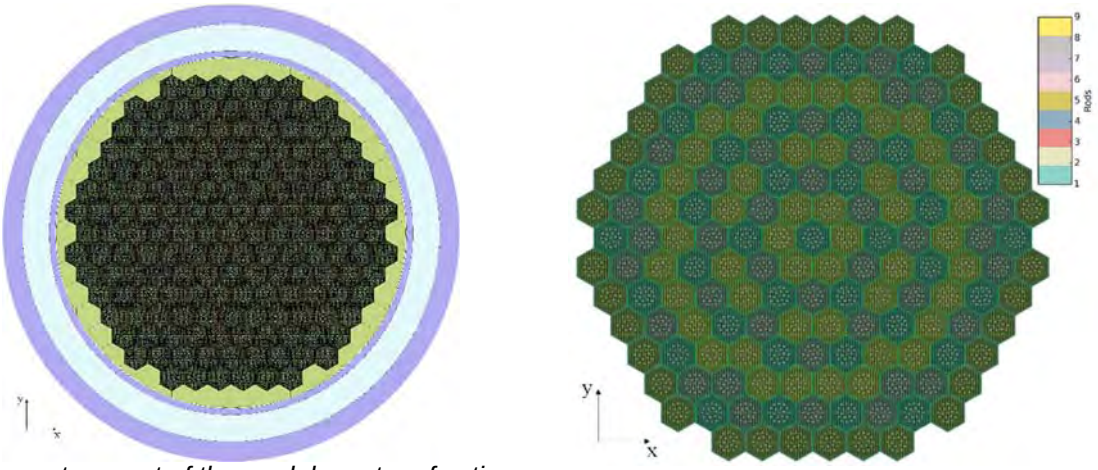


6.3 Validation for full-scale VVER

Similar excersises followed using the data from a VVER-1000 reactor with hexagonal fuel assemblies. Again, predictions of HZP criticality and control rod worths were compared to measured data. The predictions are in good agreement with measurements.

The capability of the tools within a full-scope 3D VVER case was tested through the Serpent 2 and the subchannel TH analysis of a well-known benchmark case [13]. A full scope pin-by-pin modelling was developed, as depicted in Fig. 17, where further details can be obtained from [13].

Fig. 17 Serpent 2 and SCF models for the VVER case [13]

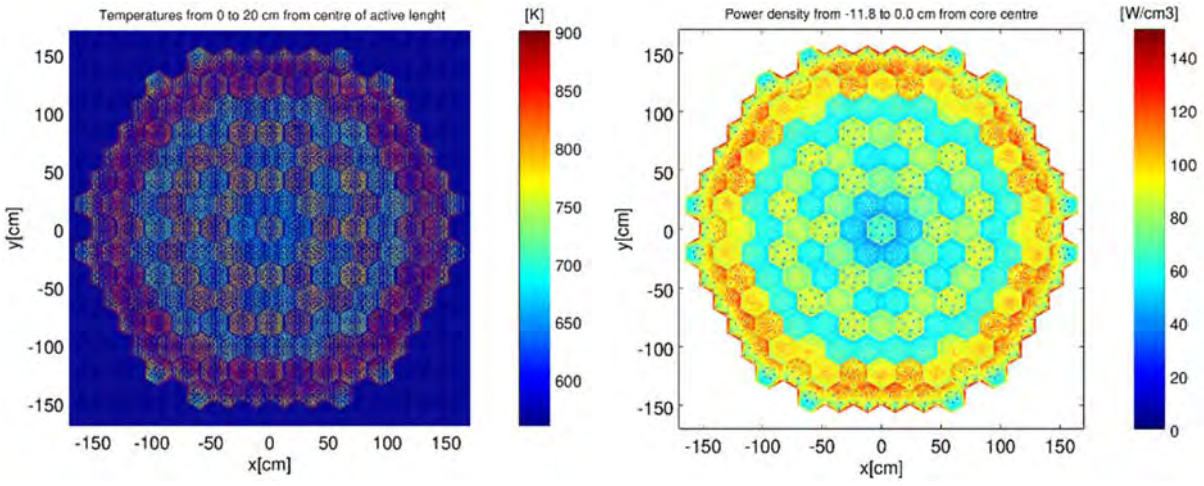


a)Serpent x-y cut of the model- center of active length

b) SCF model

Examples of the *high-fidelity* features of the approach is shown through the results obtained both for power and temperature fields, as presented in Fig. 18.

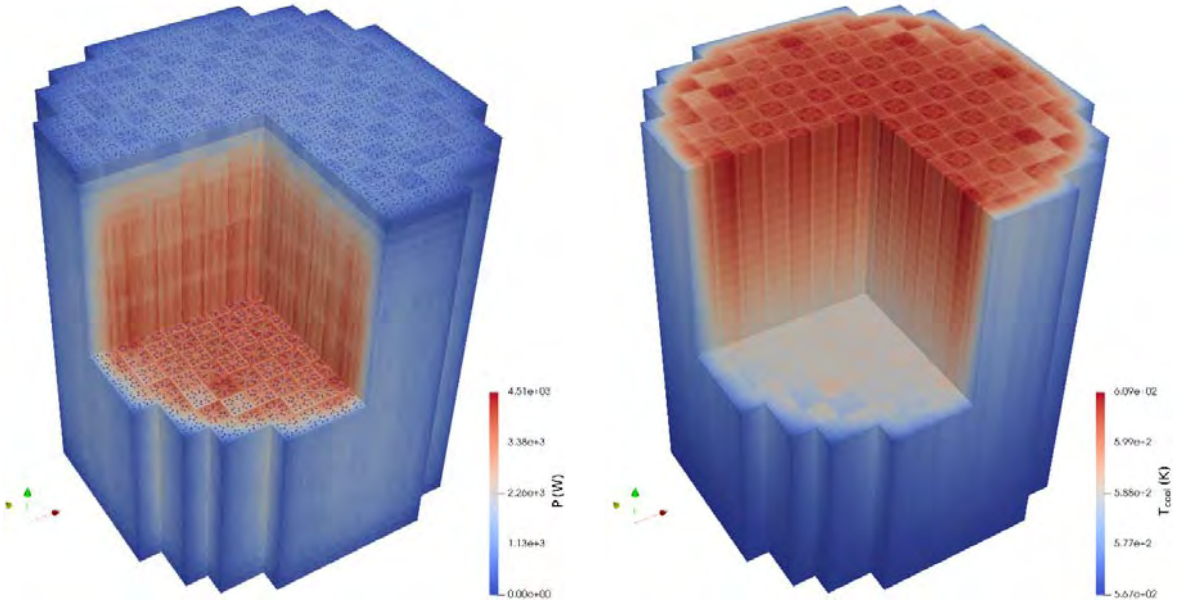
Fig. 18. Example of Serpent-SCF highly detailed results for the VVER steady-state case.



The newly developed Serpent-SCF-TU depletion capabilities are validated with experimental data from a German Pre-Konvoi PWR and a Czech VVER-1000 power plant. Within these tests the predictions of boron concentration as a function of burnup were compared to the plant data and the predicted power distributions were compared to measurements as well.These simulations are a demonstration of the cutting-edge burnup capabilities developed during the project, namely neutronic-thermalhydraulic-thermomechanic full-core pin-by-pin analysis [14].

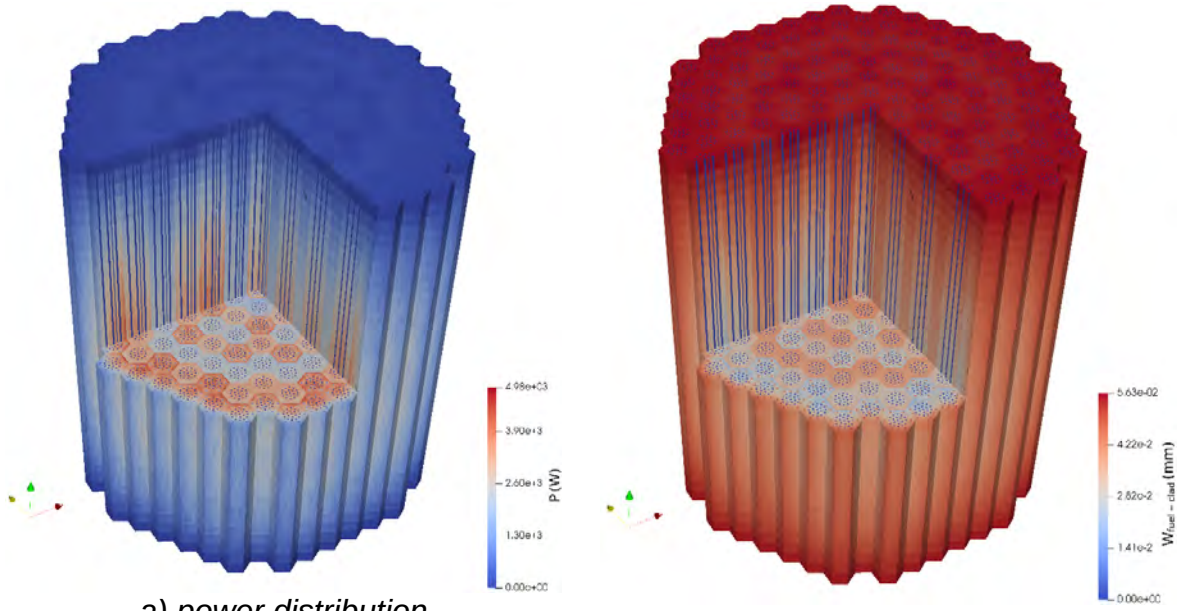
An example of these features is presented in Fig. 19 and Fig. 20 where results for these coupled full-scope calculations are presented both for PWR and VVER cases, respectively.

Fig. 19. Preliminary results for full-core PWR depletion (power, left, and coolant temperature, right).



a) power distribution *b) Temperature distribution*

Fig. 20. Results for full-core VVER-1000 depletion (power, left, and fuel-cladding gap width, right).



a) power distribution *b) Cladding gap width*

6.4 Validation for the SPERT IIIE reactor

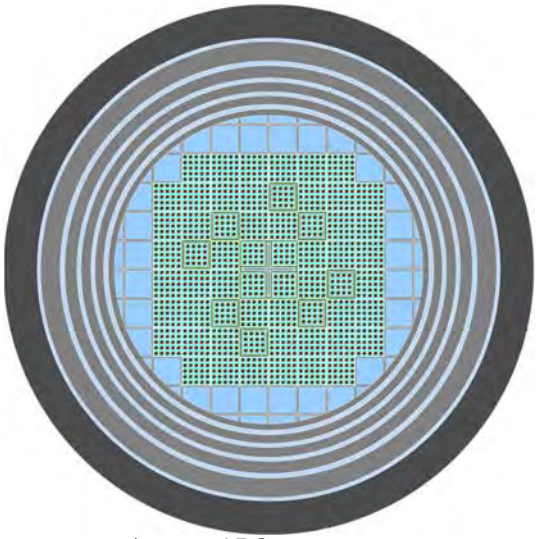
The validation of the coupled transient calculation approach based on Serpent and SCF using the experimental data from SPERT IIIE reactor was developed [15].

This SPERT III reactor was a 40 MW pressurised water research reactor, designed in the 1960s as part of the U. S. Atomic Energy Commission's reactor safety program in 1954 with diverse core designs, devoted to experimental and theoretical investigations of the kinetic behaviour and safety of nuclear reactors. In particular, the SPERT IIIE configuration consisted of an oxide fuel (pin type)

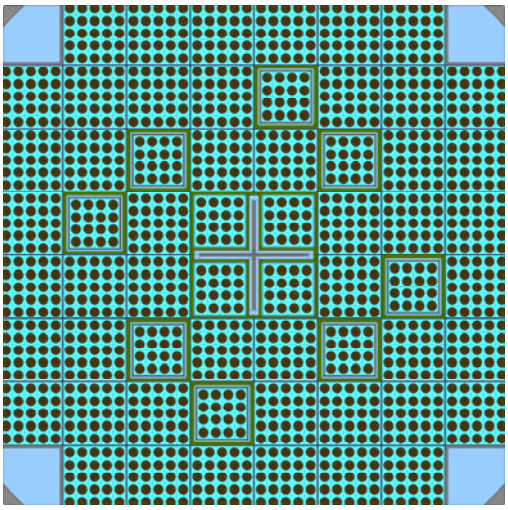
pressurised-water core, designed specifically to develop reactivity accident tests, which provided data for verification of calculation models.

Except for its small size, this reactor has the characteristics of an unborated, commercial, pressurized-water reactor (PWR), with essentially no fission product inventory in the core (it can be considered fresh fuel). Therefore, the E-core initial test conditions were representative of cold startup, hot-startup, hot-standby, and operating-power conditions in a fresh PWR. The tests were initiated with rapid reactivity insertions ranging from 0.5 to 1.3 $, which resulted in non-damaging power excursions with reactor periods from about 1000 to 10 msec. These data provide the only

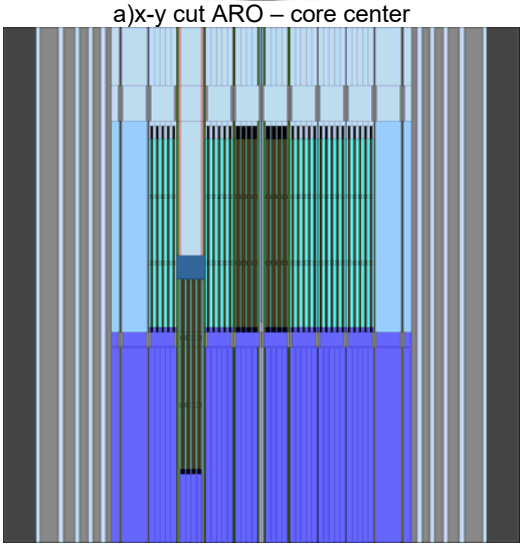
Fig. 21. Serpent 2 and SCF models



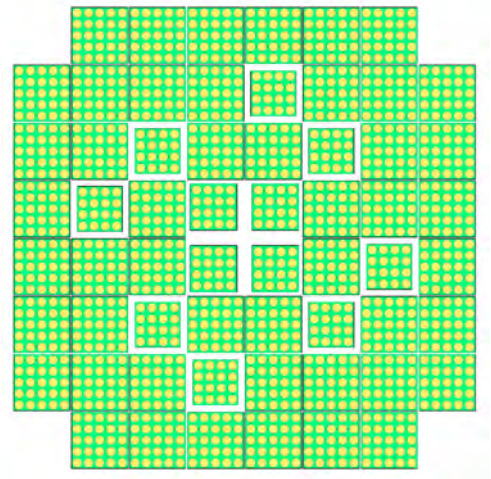
a)x-y cut ARO – core center



b)x-y cut- ARO–core center details



c) x-z cut 3.3. cm from centre - CR inserted 37cm from bottom of AL – TR inserted 2.5cm – not scale



d) Subchanflow model

known experimental reactivity accident results for low-enriched oxide cores at initial conditions other than cold-startup.

Proper Serpent and SCF models were built, as depicted in Fig. 21, where details can be directly gathered in [15]. These models were used to calculate two RIA-kind transients developed during SPERT-IIIE experimental campaign (namely T-84 and T-85), which will be presented here.

The coupled modeling considered 20 axial zones, where no explicit modelling of the axial displacement of CR is included for the interchange of power and TH fields from/to Serpent. As a result, to tackle this CR movement, the mapping to IFC is done through and ad-hoc mapping file

obtained from the SCF preprocessor, which considers the CR position and thus maps the power and TH fields.

The obtained main results are shown in Fig. 22 including the comparison with experimental values, where a very good agreement is observed. On top of that, the high-fidelity features of the approach are shown in Fig. 23 and Fig. 24 through the evolution of the power and temperatures fields evolution for the scenario T-85, where the consistency can be assessed.

Fig. 22. Main results for Test 84 and 85 - Stdev at 2σ

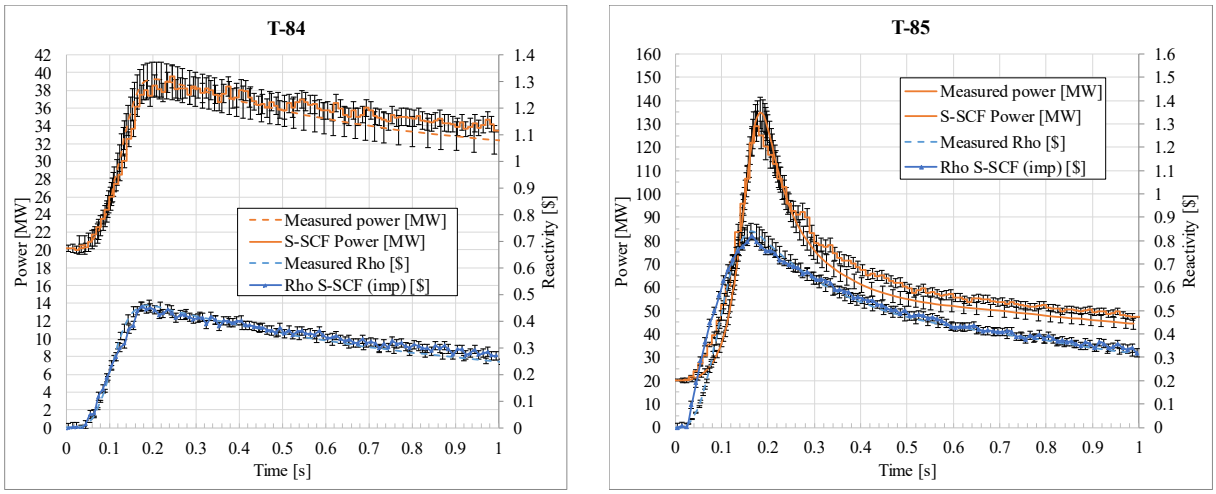
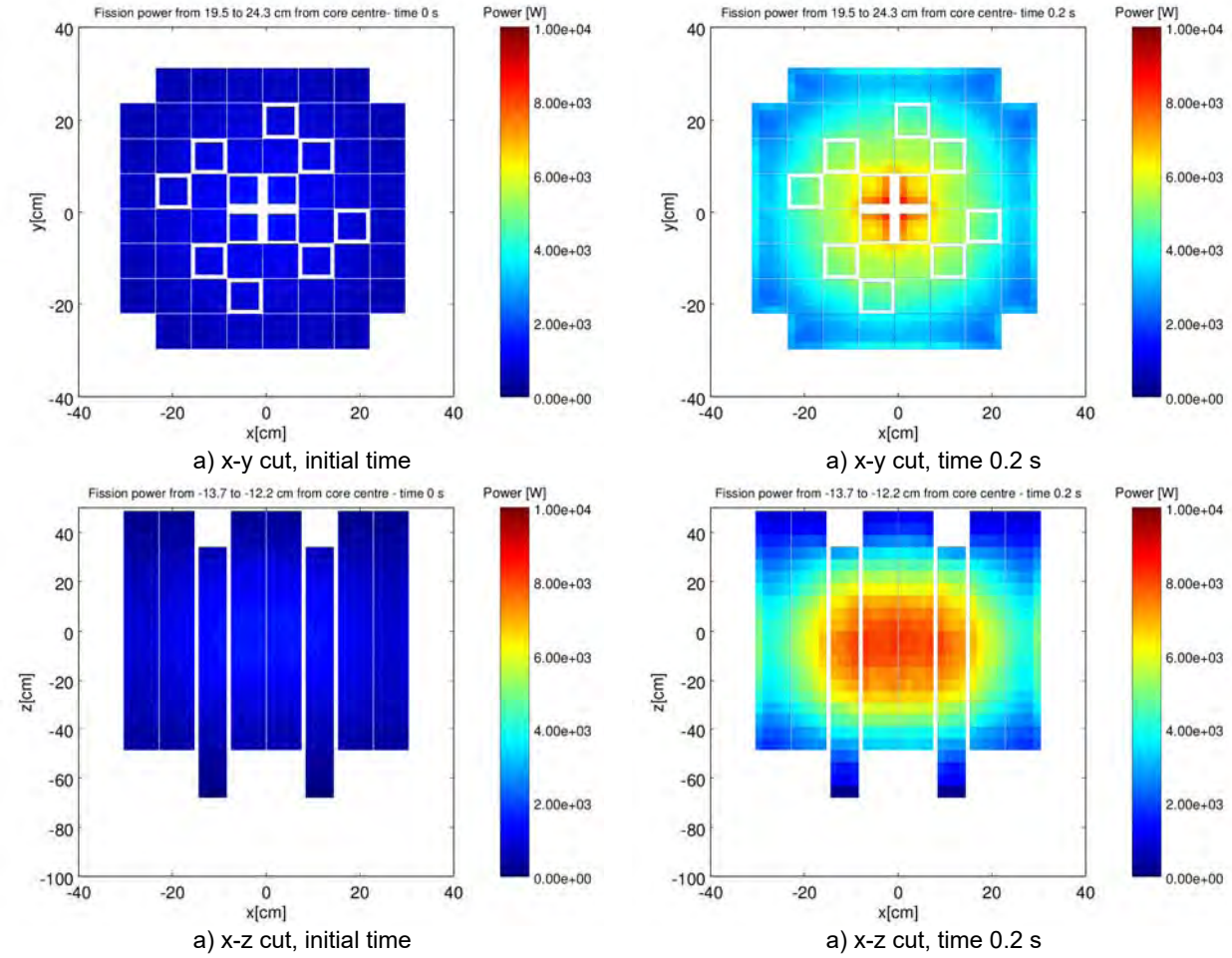


Fig. 23. Serpent-SCF power evolution for Test 85



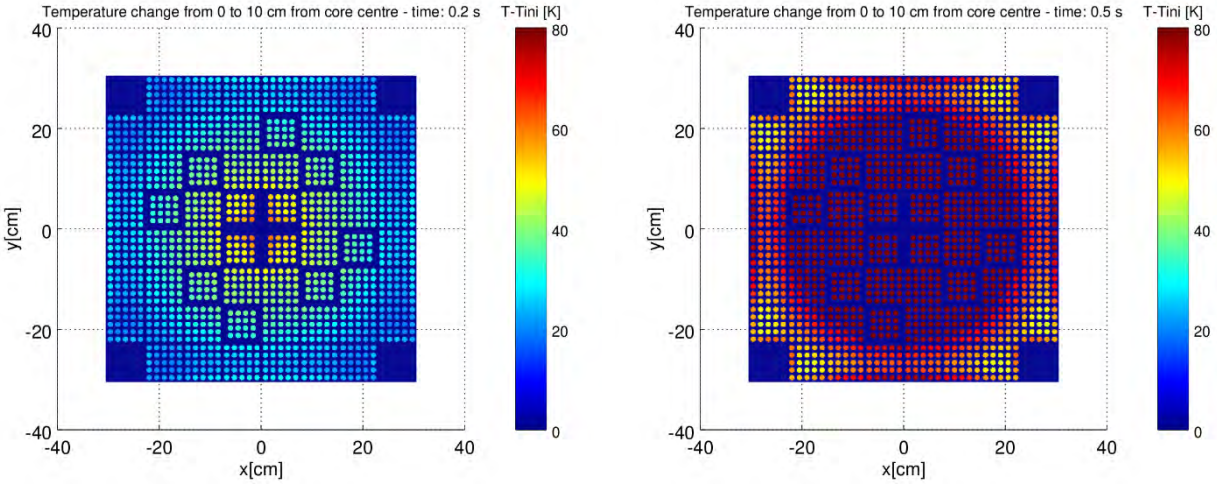
a) x-y cut, initial time

a) x-y cut, time 0.2 s

a) x-z cut, initial time

a) x-z cut, time 0.2 s

Fig. 24. Serpent-SCF temperature evolution results for Test 85



a) x-y cut, 0.2s

b) x-y cut, 0.5s

In the last year of the project, CEA has also validated the dynamic simulations against the experimental datasets available for the reactor power excursions of the SPERT III E-core. A neutronics model for TRIPOLI-4® has been built and thoroughly verified. A reliable thermal-hydraulics model for this reactor core has been developed in conjunction with KIT, based on the SUBCHANFLOW code. By following the specifications previously discussed with the other partners of the McSAFE project, we have selected a few representative RIA-like power excursions of the SPERT-III E-core, namely test T-84 and T-85. The former consists of injecting about 0.5 $ reactivity by a rapid extraction of the central transient rod, whereas the latter consists in injecting about 0.9 $; in both tests, the injected reactivity is compensated by the thermal-hydraulic feedback: the Doppler effect and the moderator temperature effect. As fiducial quantities, we have compared the power profiles as a function of time as computed by TRIPOLI-4® coupled to SUBCHANFLOW to the available experimental measurements.

Simulation results show a fully satisfactory agreement (within experimental and statistical error bars) with respect to measured data, which supports the validation of the new kinetic solver and of the multi-physics interface. For illustration, the power excursions for the two tests and the spatial shape of several computed physical observables during test T-85 are given in Figs. 23, 24 and 25. These results will be shortly submitted to a journal.

The simulations reported here are extremely time-consuming (13k CPU hours) and have thus been carried out by resorting to parallel calculations. In the context of the McSAFE project, the native (distributed) parallel simulation scheme of TRIPOLI-4® has been extended in order to accommodate the dispatch of updated temperatures and densities across the processors.

Fig. 25. Total reactor power as a function of time during the T-84 transient experiment, as calculated by TRIPOLI-4/SUBCHANFLOW, for an initial reactor power of 19 MW (blue) or 20 MW (green). The yellow line corresponds to a 19 MW calculation with sudden withdrawal of the transient rod. Statistical error bars (one standard error) are shown. All the calculation results have been shifted forward in time by 70 ms.

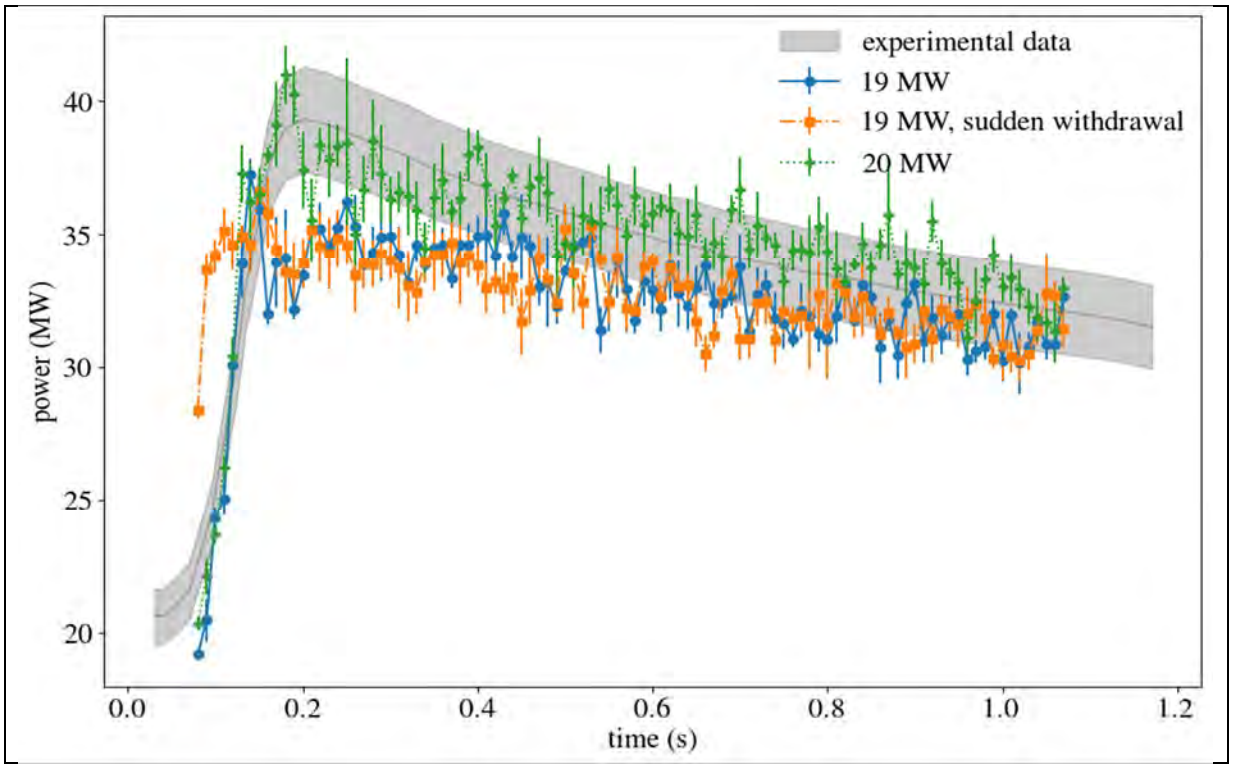


Fig. 26. Total reactor power as a function of time during the T-85 transient experiment, as calculated by TRIPOLI-4/SUBCHANFLOW, for an initial reactor power of 19 MW (blue) or 20 MW (green). The yellow line corresponds to a 19 MW calculation with sudden withdrawal of the transient rod. Statistical error bars (one standard error) are shown. All the calculation results have been shifted forward in time by 70 ms.

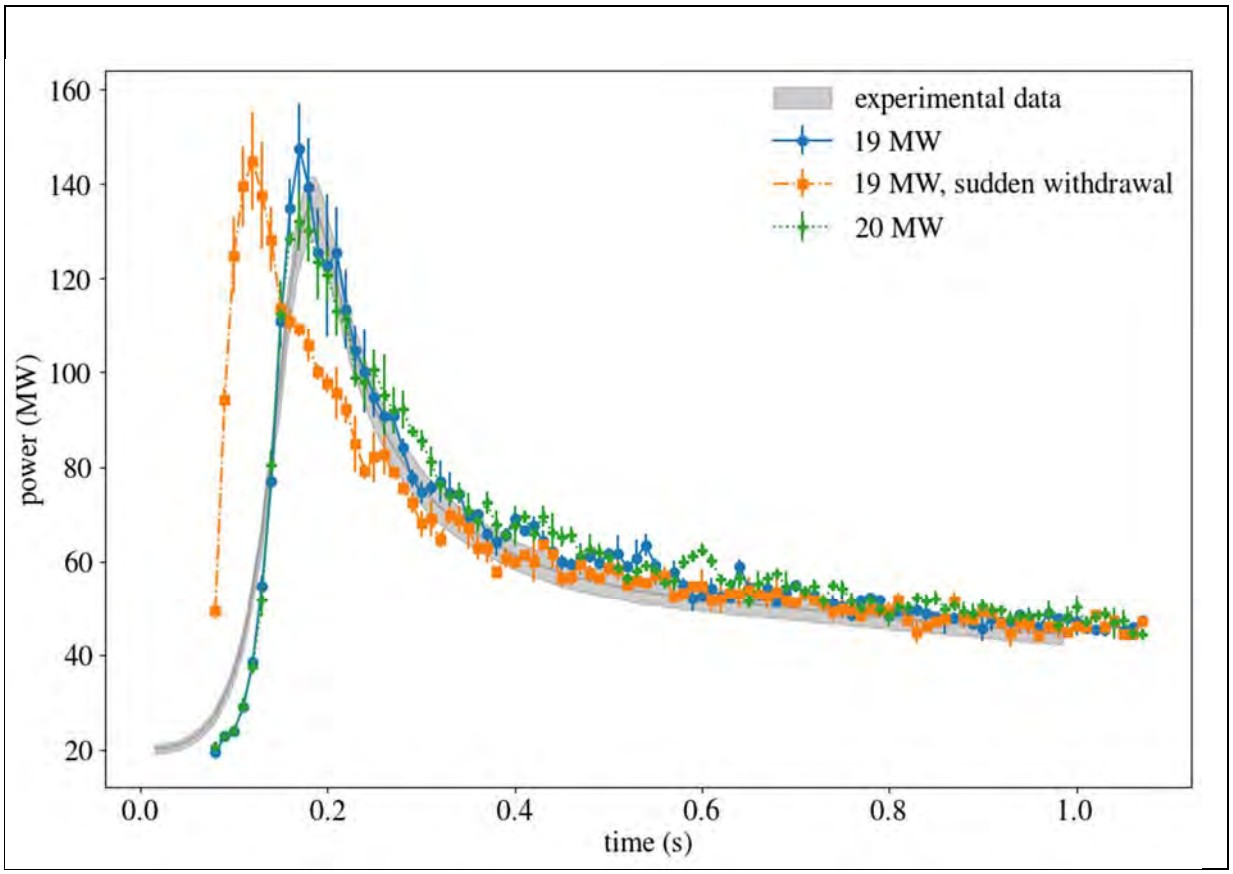
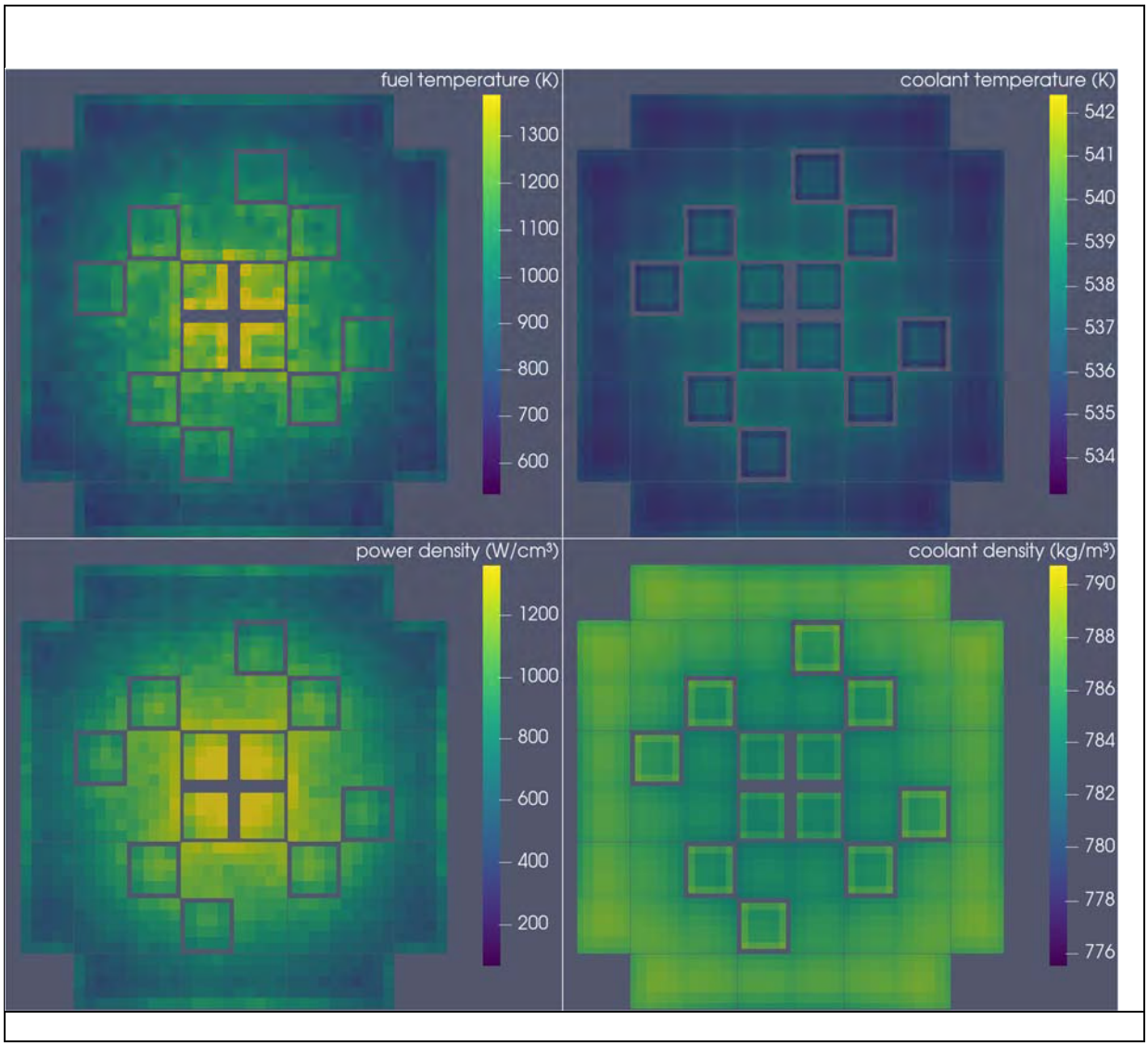


Fig. 27. Radial cuts of the fuel temperature (top left), coolant temperature (top right), power density (bottom left) and coolant density (bottom right), as calculated by TRIPOLI-4/SUBCHANFLOW, for the 20 MW T-85 transient experiment (control rods at 14.30 cm, transient rod at 16.40 cm) between t = 160 ms and 170 ms. The plane represented in the plots lies at 30.8 cm from the bottom of the core.



6. Conclusions

The current synthesis report, together with the first and second synthesis reports, show that the major goals of the McSAFE project have been realised in due time. The validation calculations for different reactor types show that reliable high-fidelity result are obtained with the developed codes and code combinations for industry-like aplications.This includes static calculations with thermal-hydraulic and thermo-mechanical feedback, depletion calculations, and calculations of dynamic transients with thermal-hydraulic feedback due to control rod movement.

This was only possible due to the extensive underlying improvements in the Monte Carlo codes like advanced depletion schemes, improved variance reduction, improved scalability for parallel processing as well as development of time-dependent Monte Carlo calculations and many other

detailed improvements. The development of an efficient coupling scheme of the various types of codes is also a corner stone for the proper execution of the validation calculations.

The progress is regularly communicated with all interested parties via newsletters, synthesis reports, presentations at international conferences and articles in scientific journals.

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