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REDUCTION OF RADIOLOGICAL ACCIDENT CONSEQUENCES

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Abbreviations

ACRR	Annular Core Research Reactor
AI	Artificial Intelligence
ANL	Argonne National Laboratory
ANN	Artificial Neural Network
APROS	Advanced Process Simulation Software
ARTIST	AeRosol Trapping In Steam generator
ASTEC	Accident Source Term Evaluation Code
ATHLET	Analysis of Thermal Hydraulics of Leaks and Transients
ATF	Accident Tolerant Fuel
BEPU	Best Estimate Plus Uncertainties
BIP	Behaviour of Iodine Project
BWR	Boiling Water Reactor
CD	Core Degradation
CIAU	
COCOSYS	COntainment COde SYStem
CRL	Chalk River Laboratories
DBA	Design Basis Accident
DEC-A	Design Extension Conditions-A
FRAPCON	Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup
FRAPTRAN	Computer Code for the Transient Analysis of Oxide Fuel Rods
FSCB	Full Scale Containment Blowdown experiments
EPR	European Pressurised Reactor
FP	Fission Product
FG	Fission Gas
HBS	High Burn-up Structure
IAEA	International Agency for Atomic Energy
LB	Large Break
LOCA	Loss Of Coolant Accident
LOFT	Loss of fluid test
MC	Monte Carlo
MFPR-F	Model for Fission Product Release - France
NEA	Nuclear Energy Agency
NPP	Nuclear Power Plant
OECD	Organisation for Economic Co-operation and Development
ORNL	Oak Ridge National Laboratory
PBF	Power burst facility
PRISE	PRImary to Secondary leak accident
PWR	Pressurized Water Reactor
RC	Radiological Consequences
RCS	Reactor Coolant System
RING	Release of Iodine and Noble Gases
SGTR	Steam Generator Tube Rupture
STEM	Source Term Evaluation and Mitigation
TH	Thermal-Hydraulics
THAI	Thermal-hydraulics, Hydrogen, Aerosols and Iodine
VVER	Vodo Vodianoï Energetitcheskyi Reactor
WP	Work Package

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1 Introduction

The R2CA 4-year project, dedicated to the Reduction of Radiological Consequences of Accidents, was intended to improve the methodologies for assessing the environmental radiological sources terms of accidents within design basis and design extension conditions. It focussed on two main kinds of accidental scenarios (LOCA & SGTR) and covered a wide range of LWR concepts (PWRs, EPR, BWR & VVERs). More especially its main goals were:

- To provide more realistic evaluations of the radiological consequences (then the safety margins) of the two categories of selected accidental scenarios within the Design Basis (DBA) and Design Extension (DEC-A) domains for different kinds of LWR concepts.
- To increase the NPP safety levels through optimizations of their emergency operating procedures, the development of innovative methods (based on artificial intelligence) for anticipated diagnosis/prognosis of specific accidental situations and more accurate evaluations of the pro and cons of Accident Tolerant Fuels (ATF) promoted worldwide.

To meet these objectives the following mains actions have been planned:

- Built a dedicated database gathering existing experimental data of interest for the accidental scenarios and conditions of interest to be used to verify and calibrate the updated/improved models or tools developed during the project.
- Make a comparative assessment of the existing methodologies used in different countries to evaluate the radiological consequences of LOCA & SGTR as well as of the associated assumptions/hypotheses,
- Evaluate the capabilities of different kinds of simulation tools (i.e. integral or detailed codes) used within the project to model the key phenomena for the source term evaluation of LOCA & SGTR and identify potential areas for improvements.
- Provide upgraded simulation tools and calculation methodologies allowing to reduce the degree of conservatism and minimize the use of decoupling factors in radiological source term evaluations able to derive more realistic safety margins for LOCA & SGTR accidents within DBA & DEC-A domains.
- Formulate recommendations for more realistic calculation methodologies of LOCA and SGTR radiological source terms (then radiological consequences) within DBA & DEC-A conditions applicable for different kinds of operating and foreseen reactors in Europe.
- Take advantage of the upgraded calculation methodologies to optimize some Emergency Operating Procedures and more accurately assess the safety benefits of new concepts developed or under development today (such as for LOCA the Accident Tolerant Fuel).
- Develop innovative methods/tools based on Artificial Intelligence (such as Neural Networks) and demonstrate their ability to provide a reliable early diagnosis of some accidental scenarios.

Reducing some of the conservatisms and decoupled factors currently used in safety studies or licensing calculations to provide more realistic evaluations of the radiological consequences of accidental DBA/DEC-A scenarios and of their associated safety margins is important to cope with and anticipate the potential changes to come in NPP operating conditions (e.g. the increase of fuel burn-up, the progressive use of new types of fuel such as ATF…). It's also particularly important to be able to extend with confidence these evaluations to other types of NPP concepts in the context of the current worldwide interest for developing new reactor concepts such as SMRs for which realistic radiological source term assessments will be even more crucial due to their potential proximity to homes and population.

Meanwhile, in the current context of increased deployment of the nuclear industry worldwide and the construction of new reactors with enhanced safety, the necessity to have a better understanding of the evolution of accidental scenarios (to be aware of their potential consequences and to evaluate the potential associated source term and/or to prevent or mitigate the source term amount) also lead to the need from the need to dispose of, search for and/or innovative devices, tools and procedures. Various computation tools and expert systems are already used for accident management/emergency operating procedures (such as optimisation algorithms, symptom, or event- based…allowing the optimisation of the selection and use of AMP/EOP that are available for an operator during the accidental transient) and their use is set to extend to even more complex problems as their computational capabilities increase. Otherwise, a promising but still challenging approach which is in a continuous development to analyse and reduce the RC of accidents, is machine learning methods (such as methods based on neural networks…).

All these topics have been the subject of specific activities and work performed within the project structured into the four main following technical work-packages, the main objectives of which are recalled below:
:

- WP2-METHOD: perform two successive set of reactor calculations analyzing to evaluate the safety margins of both LOCA and SGTR scenarios within DBA and DEC-A conditions and make recommendations for a harmonization of the calculation methodologies for the evaluation of their radiological consequences (RC).
- WP3-LOCA: develop accurate simulation tools & calculation schemes for the evaluation of the RC of LOCA scenarios by improving the existing tools for both accidental progression in the core and release/transport of fission products up to the environment.
- WP4-SGTR: develop accurate simulation tools & calculation schemes for the evaluation of the RC of SGTR scenarios by improving the existing tools for both accidental progression and release/transport of fission products up to the environment.
- WP5-INNOV: identify and evaluate the gains using the updated simulation tools of potential new accident management procedures/devices including Accident Tolerant Fuels and explore the capabilities of Artificial Intelligence functionalities for anticipating accidental configuration through an early diagnosis of fuel rod defects.

The main outcomes and achievements for each of these topics obtained during the project are summarized in this report. In addition are also reported the main activities and results of the work package dedicated to communication, education and training, dissemination (WP6).

2 R2CA project overview

This section gives a brief overview of the main advances made during the project, whether in terms of developing/improving models, simulation tools and/or calculation chains, or the impact of these modifications on the re-assessments of the radiological consequences of LOCA and RTGV accidents within DBA and DEC-A conditions. A summary of the main work carried out in terms of innovation is also presented, concerning the use of innovative computational methods (based on algorithm optimisations, expert systems, machine learning methods…) for Emergency Operating Procedure improvements and the demonstration of the capability of an early diagnosis tool for defective fuel rod detection. Finally, main communication, education and dissemination activities performed carried out during the project are listed.

The main advances and results for each work package are listed below and will be described in greater detail later.

- **WP2**: Exhaustive reviews of methodologies currently used by partners involved in the project for calculating the environmental radiological source term as well as the available models in the different simulation tools (i.e. integral or detailed codes…) for areas of interest within the project (mainly FP, fuel and clad behaviour) were performed, A specific database was also built in support of the V&V of new developed/improved models. It includes data of interest for the transient and conditions explored in the project and/or reports issued from more than 200 tests performed at different scales and NPP measurements. About 35 accidental scenarios (both LOCA & SGTR) were calculated on different kinds of reactor designs (VVERs, PWRs, EPR and BWR), covering both DBA and DEC-A conditions. Two sets of calculations were provided (i.e., 70 calculations): the initial with the existing methods/calculation tools and chains, and the second with improved calculation chains incorporating the improvements developed in WP3 and WP4. The impact of new modelling was clearly evidenced through the comparison of their environmental activity releases and radiological consequences: in most cases, the improved calculations led to fewer released activities in the environment and then lower radiological consequences thanks to reduced conservatisms (in assumptions, model parameters…) and avoiding the use of decoupling factors. Datasheets for each calculation were provided which can be further use for a database creation. Finally, some sensitivity analyses and uncertainty quantification were also performed providing information on where the future developments should be focused on. All these results and their analyses served as a sound basis for formulation of generic recommendations in Radiological Consequences evaluation for methodology harmonisation. Finally, regarding uncertainty quantification a global approach combining uncertainty of single calculations when used in a coupled mode was proposed. However, no systematic uncertainty analyses were performed within the project as much more time/effort than devoted to the project would have been necessary. Some work has nevertheless been carried out (incl. sensitivity analyses for identification of important parameters, specific extension of some codes to perform these analyses, extended application of the CIAU methodology to environmental iodine releases in SGTR).
- **WP3**: Several model improvements/developments involving different modules in calculation chains were performed. Calculations chains were also updated and for existing models a dedicated V&V work for the specific DBA & DEC-A conditions was carried out. The main developed/improved models that have been performed are listed below by category: FP in primary circuit/containment, clad T/M behaviour and burst, Fuel T/M behaviour and FP releases.
  <u>FP transport & in-containment behaviour:</u> only few improvements were done. It concerned iodine/paint interaction model in COCOSYS where an update was performed to better account for VVER types of paints.
  <u>Fuel T/M behaviour & FP releases:</u> the work was focussed on enhancing the coupling between fuel performance code (TRANSURANUS) and mesoscale/grain scale FP codes (SCIANTIX & MFPR-F) and improving/developing models in these codes (incl. more mechanistic modelling of the High Burn-Up structure evolution, transient FP releases due to stress/power variations, axial gas communication in fuel rod that should allow a better prediction of the clad ballooning and burst failure risks). More detailed

calculations of the fuel gap inventory (incl. a 3D burn-up calculations for VVER fuel types) were also provided.
Clad T/M behaviour & burst: new burst criteria (in T, stress & strain) more appropriate to DBA & DEC-A conditions were built and tested vs DRACCAR and FRAPTRAN test cases. Upgrades of cladding deformation models for E110 clad material and of transformation phase model for M5 clad material were also proposed in FRAPTRAN & TRANSURANUS.
Regarding calculation methods used to calculate the number of failed rods, the available statistical methodologies were checked and applied for reactor concepts analysed in the project. New calculation methods, using a detailed 3 D thermal-hydraulic core modelling at a fuel assembly scale and an integral code coupling thermal-hydraulic to fuel rod thermomechanics were also investigated (with DRACCAR and ATHLET-CD) more suitable to capture the 3D heterogeneities in ac ore due to non-symmetrical heat-up during a LOCA but also to heterogeneities in fuel assembly power distribution and location.

- **WP4**: As for WP3 several model improvements/developments involving different modules in calculation chains were performed. Calculations chains were also updated and for existing models a dedicated V&V work for the specific DBA & DEC-A conditions was carried out. The main developed/improved models that have been performed are listed below by category: FP transfer from primary to secondary circuit, clad secondary hydriding, Fuel T/M behaviour and FP releases.
  FP transfer from primary-to-secondary circuit: enhancements of T/H code capabilities for FP transport simulation in the primary circuit (incl. dilution, removal effects…) were performed as well as extension/upgrading of the integral code capabilities (i.e., MELCOR…) to simulate specific phenomena occurring in failed SG (i.e., flashing, atomisation, partitioning, scrubbing…)
  Fuel T/M & FP releases: the work was focused on enhancing the prediction of the “spiking” FP releases from defective fuel rod gap due to transient conditions (i.e., power transients…). Several improvements/developments of models were performed either in T/H codes (i.e., RELAP5…) or in dedicated codes (i.e., RING….) or in integral codes (i.e., in MELCOR, MAAP…) with the implementation of external functionalities integrating more physic-based modelling (i.e., enhanced diffusion and forced convection releases). Improvements mainly concerned iodine. In addition, some model improvements were also performed in fuel performance codes (i.e., TRANSURANUS) and in FP behaviour codes (i.e., in SCIANTIX) (incl. fuel oxidation, FP release dynamics during power transients…).
- Secondary hydriding of defective rod clad in normal operation conditions: new tests on H_2 uptake by Zr_4 and E110 were performed. The results were shared within the project and used for the refinement of H_2 uptake models. Developments of integral models related to clad secondary hydriding from water ingress to hydride blister formation (incl. gas diffusive mixing and transport in fuel rod gaps, clad hydriding, H_2 radial re-distribution, hydride precipitation/dissolution…) and implementation in multi-physics tools (i.e., FRAPTRAN, SHOWBIZ…) were performed.
- **WP5**: An optimisation of the Accident Management/Emergency Operating Procedures was done mainly dedicated to VVER 1000 concepts and SGTR scenarios. Different methods were used (incl. the SIMPLEX event-based method…) and PRISE scenarios analysed for optimisation of actions and/or set points leading to a reduced activity released in environment and increased grace times for operator’s actions to be done. In addition, a promising prototype of ANN-based tool for detection and characterization of defective fuel rod in normal reactor operating conditions was developed and tested. Finally, evaluations of some ATF concepts (mainly Cr-coated Zr, FeCrAl, U3Si2, Hastelloy-n) were performed using different tools (DRACCAR, TRANSURANUS, FRAPTRAN...) and some sensitivity and uncertainty analyses performed. Some of them used updated tools developed during the project (i.e., evaluation of Cr-coated Zirconium-based clad thermomechanical behaviour with the updated DRACCAR tool…). The impact of new material properties on the fuel performance (i.e., delay in clad burst timing…) were highlighted through SA & UQ analyses or, for Cr-coated Zr through recalculation of experimental cases (QUENCH L1, QUENCH LOCA, IFA -650…).
  In parallel several bibliographical studies and literature surveys were also carried out in each of the tasks of this WP which have fed into the different WP activities. In particular, they were used to identify the main requirements for developing advanced devices and/or accidental management procedures (e.g. algorithms for SGTR management in VVERs, to identify the pro/cons of using Artificial Intelligence for

NPP accident analyses, to review existing defect diagnosis tools and AI techniques dedicated to fault detection in non-nuclear fields, and finally to select the generic thermophysical/chemical properties (i.e. thermal expansion, diffusivity, conductivity, heat capacity...) needed for the performance evaluation of Advanced Tolerant Fuel with coated Zr clads.

- **WP6**: Regarding result dissemination and communication activities, 4 newsletters were issued (one per year reporting on major advances), 18 presentations (general or more specific ones) were made in International/National conferences (incl. NENE, TOPFUEL, NURETH, ERMSAR….), 6 papers published in peer-reviewed journals (incl. Journal of Nuclear Materials, Nuclear Engineering and Design, Progress in Nuclear Energy…), and a R2CA special issue of Annals of Nuclear Energy initiated with a total of 18 papers. The 15 public technical deliverables issued from WP2 to WP5 were or will be also archived in Zenodo in a dedicated R2CA project community folder and shared through social networks and R2CA public website. Regarding Education & Training, 3 code trainings (dedicated to DRACCAR, TRANSURANUS and SCIANTIX) and one summer school (dedicated to DBA and DEC-A accidents for LWRs) were organised. Four mobilities were carried (slightly reduced compared with initial plan due to Covid-19 issues). Also 1 post- doctoral, 1 PhD and 5 MSc students participated in and contributed to the project.

3 R2CA database

The experimental data on reactor incidents and accidents built within the project [1] provided the basis for code validation and development activities and served as the background of current knowledge on related phenomena. The EU R2CA review of experimental databases covered more than forty experimental series including thousands of tests, which characterizes the phenomena taking place during LOCA and SGTR events in PWRs and VVERs. Among the tests several separate effect tests and integral tests are listed, and some NPP measurements were also included.

- Fuel failure during LOCA is well covered by experiments, since many test series have been carried out under different conditions with all important cladding types. In addition to burst type failure – which took place in more than twenty reviewed test series –, the brittle failure of Zr alloy claddings due to thermal and mechanical loads was observed in some tests. The fuel pellet fragmentation and dispersal were indicated by several tests (PBF, FR-2, ACRR, ANL, FLASH, Halden LOCA, Studsvik LOCA).
- Fuel failure during SGTR normally is not expected for intact fuel rods. The related experiments simulate the behaviour of defective fuel rods, which may suffer from secondary defects during the accident. The available experimental data characterise the hydrogen uptake by Zr alloys in the defective fuel rods and its embrittlement effect.
- Activity release from fuel during LOCA conditions was simulated in several separate effect tests (HEVA, VERDON, VERCORS, GASPARD, ITU FP, ORNL FP and CRL FP) and also by integral tests (ACRR, FLASH, Halden-LOCA, LOFT LP-FP). The available experimental data cover a wide range of parameters for different fission products. The Halden fission gas release (FGR) tests are also important for this topic, as they may provide part of the gap source term in case of fuel failure.
- Activity release from fuel during SGTR conditions is supported by iodine spiking experience at PWR and VVER NPPs and by separate effect tests on leaching of fuel pellet samples. The DEFECT, DEFEX and CRL defective fuel rod test series simulated the behaviour of defective fuel rods in research reactor conditions and provided valuable information on secondary defects and water-logged fuel rod phenomena.
- Activity transport during LOCA includes several phenomena in the primary circuit and containment, which were investigated in the VERCORS, VERDON, BIP, THAI and STEM projects. The ARTIST project focused on aerosol trapping in steam generators. Some important data can be drawn from the OECD-IAEA Paks fuel project and from the Rivne NPP event with non-closure of pressurizer safety valve.
- Activity transport during SGTR is characterised by complex path configurations, which were studied in the VERCORS, VERDON, BIP, THAI, ARTIST and STEM projects. The BIP, MARVIKEN FSCB and STEM test series simulated fission product transport in the steam generator, too. The primary-to-secondary transport

phenomena were also observed in the Doel and Rivne NPP events with steam generator tube rupture and collector cover lift-up, respectively.

The experimental data were used for the support of R2CA tasks in several areas including model development and validation activities:
- burst tests' data were used for the improvement and validation of DRACCAR, TRANSURANUS and FRAPTRAN transient fuel behaviour codes,
- integral LOCA tests were used for the further validation of DRACCAR, TRANSURANUS and FRAPTRAN transient fuel behaviour codes,
- FP test data were crucial for the testing of fission gas release model in fuel behaviour codes TRANSURANUS, SCIANTIX and MFPR-F,
- FP transport experiments provided unique possibilities for the validation of numerical models used in ATHLET-CD, ASTEC, COCOSYS, SOPHAEROS and APROS codes,
- iodine spiking data were used to develop and improve activity release models applied in SGTR analyses in computer codes MELCOR, RING and TRANSURANUS,
- hydrogen uptake data were useful for the simulation of secondary degradation in defective fuel rods in the SHOWBIZ and FRAPCON codes.

The common use of data from small scale separate effect test and integral tests provides possibilities for the improved simulation of several phenomena (e.g. cladding burst, oxidation, hydrogen uptake, activity release and transport) under very different conditions. Most of these conditions can be considered as typical for LOCA and SGTR events, and some of them cover even wider parameter ranges than those that could be expected in the analysed accidents.

The reviewed experimental series were executed mainly with such materials, which are used today or were used earlier in the NPPs. In order to support the introduction of new fuel types and accident tolerant fuel designs, some of the test series could be repeated with new materials, or new experimental programs could be launched to investigate their behaviour under LOCA and SGTR conditions.

4 Main Progresses in LOCA modelling

LOCA-type accident under DBA and/or DEC-A conditions (i.e. without significant degradation of the fuel rods in the core), successively involves the fuel clad ballooning and burst, the release of the gap fission product inventory of burst fuel rods, their transport from the primary circuit to the containment, and their time-dependant physicochemical behavior in the containment before eventual release into the environment.
Different approaches can be used to evaluate the source term for this type of accident, where a good prediction of the number of burst fuel rods and of the in-containment FP source term and evolution is crucial if we are to assess their consequences more realistically. The main model improvement work carried out during the project focused on the primary circuit source term (i.e., fuel rod behaviour: gap FP inventory and FP releases from fuel), the fuel rod burst and the in-containment FP behavior.

4.1 Fuel rod behaviour

The aim was to extend the knowledge and ability of simulation codes to predict the complex fuel behaviour during a LOCA transient. Among other items, it concerned:
- The fission gas release causing additional cladding internal loading,
- The quantity and nature of radionuclides released within LOCA conditions (including rapid transients, high temperature and consideration of the high burnup structure),
- The impact of oxidation on fission gas release.

Main achievements of this work are a higher degree of mechanistic modelling has been successfully implemented in the fuel performance codes, along with an improved viscoplastic model of the cladding. More details are covered in project deliverable D3.6 [2]). The final status covering both code improvements/extensions and model verification & validation can be summarized as follows:

a) Code extensions

Regarding the coupling of the fuel performance code TRANSURANUS with two mesoscale fuel behavior codes (MFPR-F [3] and SCIANTIX [4-6]), a considerable effort has been made to develop plug-in modules that allow for a) feedback from these codes to the integral fuel simulation, including mechanical phenomena as e.g. fuel deformation, and b) applying a re-start modification option as needed for the simulation of a LOCA following a base irradiation in a commercial NPP.

Meanwhile, the integral fuel performance code FRAPTRAN [7] has been extended in terms of mechanical modelling [8], more precisely by adapting an alternative Norton-type creep law (bias derived and included) and the bias of the cladding failure limits. The FRAPCON code [9] has also been coupled with the SCIANTIX mesoscale model [4] and tested. SCIANTIX models for fission gas behaviour have been refined by increasing numerical stability and a priori error control under transient conditions.

In addition, a prototype standalone module for simulating axial gas communication during LOCA has been developed. Its current version was used to test the explicit-implicit internal coupling of the creep and the gas flow models. It is being further tested with realistic boundary conditions transferred from the TRANSURANUS code (loose coupling). The work was started with the WWER-1000 case - for fuel supplied either by TVEL (Russia) or Westinghouse (Sweden) – but due to priority constraints and time restriction, a full coupling with the TRANSURANUS code couldn't be achieved within the timeframe of the project.

Finally, in the course of a multistage approach for evaluating fuel rod behaviour during a WWER 1000 Large Break LOCA transient, a service module for off-line interfaces to be used by the TRANSURANUS code has been developed. It made use of the reactor dynamics code DYN3D [10] and the thermo-hydraulic code RELAP [11] for pre-calculating the steady state pin power and the LOCA boundary conditions, respectively. It was demonstrated that the multistage approach for a full-core analysis allowed for assessing the number of failed rods and hence the radioactive fission product release to the primary coolant in the event of LOCA.

b) Verification and Validation

For the assessment of the modified simulation tools, a number of cases from the IFPE database maintained at the OECD/NEA [12] has been selected. They cover standalone cladding burst tests (PUZRY), two LOCA experiments of the Halden Reactor test series IFA 650, one LOCA simulation test performed by Studsvik Nuclear AB, Sweden (NRC-192), as well as 3 transient irradiation experiments at the French Siloe reactor (HATAC C1 and C2, Contact 1). The available experimental data, power histories and boundary conditions were used for verification and validation of the coupled code versions. Applying the latest version of TRANSURANUS, the LOCA cases showed a fair agreement with the outcome of the IAEA FUMAC project [13], and a small impact of the various approaches for simulating fission product behaviour [14-17] on cladding deformation and rupture (**Figure 1**). First uncertainty and sensitivity analyses for the LOCA phase of IFA 650.10 and IFA 650.11 confirmed the expected dominance of the cladding outer temperatures for calculating the deformation of the cladding up to the time of burst, and indicate the importance of cladding material properties, as creep, swelling and the elasticity module.

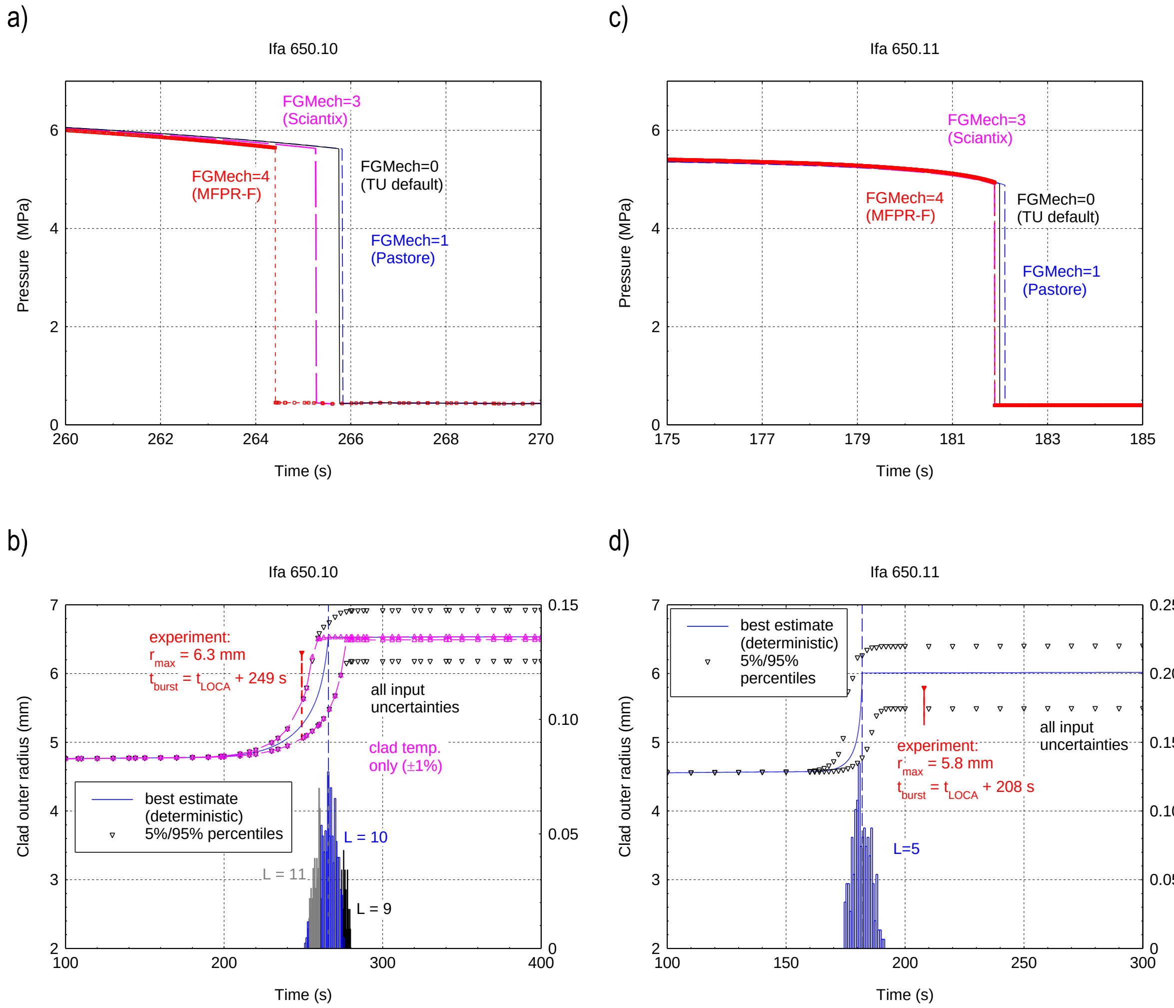

Figure 1: Inner pin pressure (a and c) and cladding outer radius (b and d - at axial location of maximum ballooning) as function of time during LOCA simulated with different options of the latest version of TRANSURANUS, for the Halden LOCA tests Ifa 650.10 and Ifa 650.11, respectively.

The extended FRAPTRAN code has also been verified using the IFA 650.10 LOCA test (**Figure 2**) and the standalone PUZRY tests. Improvements in the time-to-failure prediction are primarily linked to the viscoplastic performance of the cladding while modified failure limits will not lead to higher accuracy. A final implementation of Norton´s creep law would require the irradiation hardening effect to be included. A standalone version of the TRANSURANUS mechanical model (TUMech) has been developed for predicting the cladding response under LOCA conditions. TUmech has been coupled with FRAPTRAN-2.0 as an alternative mechanical model and the resulting tool has been validated with two Halden LOCA tests [18].

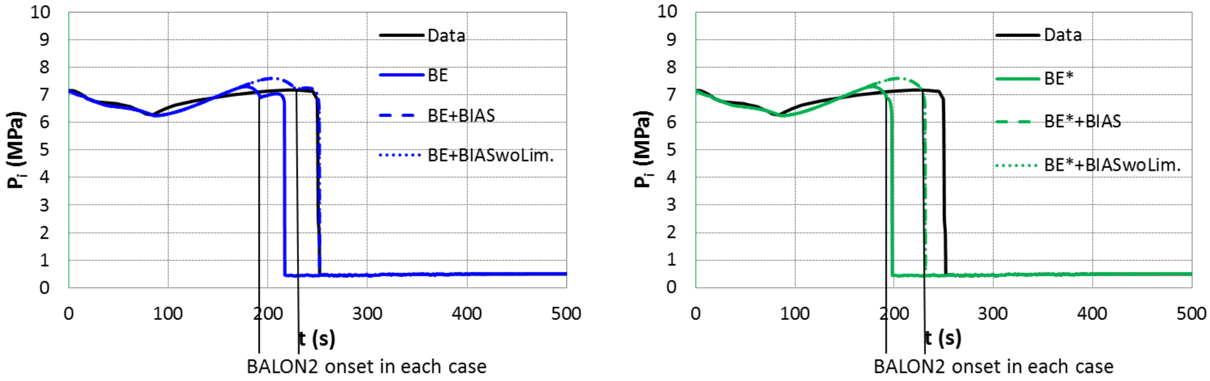

Figure 2: Model-to-data comparison for the internal pressure (P_i) in IFA-650.10 simulated with the extended FRAPTRAN code. Predictions with MATPRO´s creep model on the left and with Norton´s law on the right.

Furthermore, the code coupling TRANSURANUS//SCIANTIX has been further tested with the case HATAC C2. The current simulations tend to overestimate the release occurring during base irradiation, due to an overestimation of the release from grain boundaries predicted during power ramps and ascribed to micro-cracking of the grain faces. An uncertainty analysis using the normalized variance of the retained intra-granular Xenon concentration revealed that its maximum uncertainty is expected immediately before completing the formation of the HBS (cf. [19]).

The extension of the TRANSURANUS code for calculating local concentrations of fission product isotopes considering fission yields, decay and neutron capture [20] has been merged with the latest code version. Together with recent code extensions for ATF material properties, it has been tested for conditions of the IFA 650.10 LOCA experiment. More details are reported in Deliverable 4.4 [21].

The code coupling TRANSURANUS//MFPR-F was used for further analysis of the case NRC-192, with an updated coupling containing the HBS models of MFPR-F [22]. The prediction of fuel restructuring based on the evolution of the dislocation density was found to be satisfactory, although at present it requires to disregard the shutdown periods from the power history. Regarding the LOCA transient, FG release from the HBS zone was calculated using a model based on the pressure in a HBS pore. Although its predictions were found satisfactory, the model was empirical and could be improved by means of a more mechanistic approach.

All work related to the coupling of TRANSURANUS//MFPR-F [23] and TRANSURANUS//SCIANTIX [24] was presented at two international workshops "Towards nuclear fuel modelling in the various reactor types across Europe", 28-30 June 2021 (online) and 22-23 September 2023 (Bologna, embedded in the R2CA progress meeting). Both coupling modes are summarized in the special issue of Annals of Nuclear Energy devoted to the R2CA project [25]. It discusses the application to the LOCA test IFA 650.10 as a representative base irradiation scenario in a commercial nuclear power plant, followed by a re-irradiation in a research reactor for submission to a loss of coolant experiment, without convergence or cliff-edge effects.

4.2 Fuel rod failure & core modelling

The main objective of this work was to better evaluate the number of failed rods during a LOCA by:

- Performing fuel cladding thermomechanical data and models reassessment
- Developing different methodologies to assess the whole core behaviour during the accident.

Regarding the cladding thermomechanical modelling, three partners performed complementary work, two on FRAPTRAN and one on DRACCAR codes:

- A re-assessment of burst failure criteria was performed in order to decrease the scatter of the measured data, and the consequent re-fitting of the plastic deformation model of the code FRAPTRAN to reduce the calculation uncertainties. The first phase of the work was to study the geometry of samples of the Russian alloy E110 that underwent ballooning and burst tests. From this analysis, new burst criteria have been established and using these new criteria the parameters of the cladding plastic deformation model of the code FRAPTRAN were re-fitted.
- The FRAPTRAN code was also modified by implementing new high-temperature creep laws and dynamic crystallographic phase transformation models. New burst models from literature and developed within the frame of the R2CA project were also implemented and tested on validation test cases.
- A very large burst database was built gathering more than 1400 tests from more than twenty experimental programs on as received and irradiated rods. From these data, several burst criteria were proposed:
  - ✓ Simple envelopes on engineering burst hoop stress (min, max, mean) were fitted on the whole database (all alloys and all testing conditions) to alloy sensitivity studies (**Figure 3**).
  - ✓ A temperature criterion depending on the heating rate and the engineering stress was fitted on as-received samples internally heated. This criterion was compared to existing criteria from literature (Chapman and Meyer) and tested on several validation test cases with the DRACCAR code (**Figure 4**).

  The temperature burst criteria developed within the frame of the R2CA project are specifically dedicated to burst occurrence prediction for more accurate radiological consequence evaluation. Burst criteria on true stress and/or strain are needed for flow blockage prediction. Cladding burst is a complex phenomenon that is strongly influenced by several parameters: cladding state (i.e., hydrogen content…), inner rod volume, axial gas communication, transient fission gas release, heating mode that is highlighted by the very strong experimental results scattering. More data would have been needed (especially with irradiated fuel rods) to further develop and validate the models.

In addition, M5™ creep and phase transition models were reviewed. Results of this review have suggested to consider in more detail the model published by Massih and Jernkvist for the crystallographic phase transition and a combination of Kaddour's and Massih's models for the high temperature creep. These models have been implemented in TRANSURANUS.

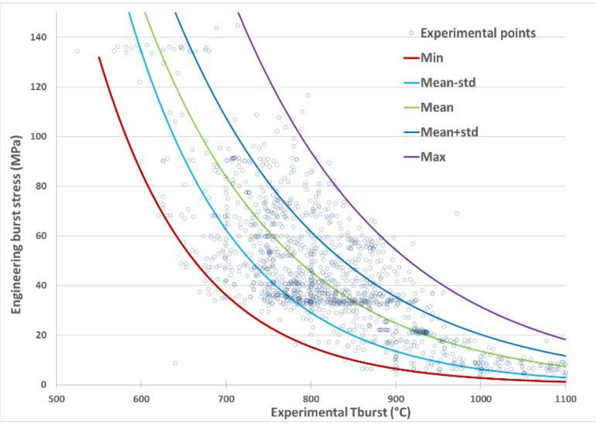

Figure 3: Engineering burst stresses vs burst temperatures: exponential models compared to experimental points from [26]

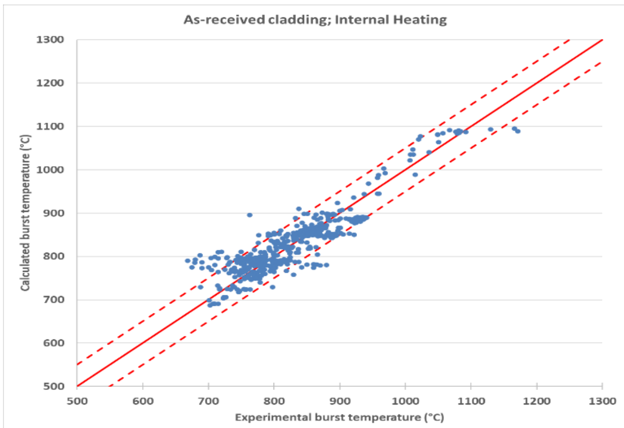

Figure 4: Calculated burst temperatures with temperature criterion vs experimental ones (dashed lines correspond to ±50°C) [26]

All work related to fuel clad thermomechanics were summarized in the special issue of Annals of Nuclear Energy devoted to the R2CA project [26]. In addition, the work dedicated to M5™ was presented at two NENE international conferences in 2021 [27] & 2022 [28].

To assess the whole core behaviour and predict the failed rod number during the LOCA transient, partners used different methodologies and core modelling. Essentially, two main approaches were selected for whole core modelling:

- Chaining system thermal hydraulic simulation to fuel performance code,
- Using integral code coupling thermal hydraulic to fuel rod thermomechanics.

During the project the 3D core modelling, part of the second approach, was more especially extended and/or developed.

The different studies and/or developments made in both approaches are described hereafter:

- **System thermal hydraulic and fuel performance code chaining**
  TRANSURANUS code was widely used, in particular for LOCA analysis in the past. The historical development and use of TRANSURANUS for LOCA and the methodology associated to fuel rod failure rate predictions was developed in EXTRA EU project. Progress has been made during the project on the statistical post-processing program TUPython [29] to support the Best Estimate Plus Uncertainty (BEPU) analyses. During the project, this method was used for a LB LOCA VVER-1000 study. It was based on TRANSURANUS simulation of rod response including the statistical treatment of the fuel rod and the code model uncertainties combined with the sensitivity study with respect to the rod power. Another calculation chain implying HELIOS, DYN3D, RELAP5, TRANSURANUS (v1m3j21) and SCALE was also applied to a VVER1000 by another partner and detailed with a specific focus on core modelling and associated input data. Calculations were performed for different rod relative power and the nature of the dependence of the number of failed rods for different moments of the cycle was assessed (**Figure 5**).

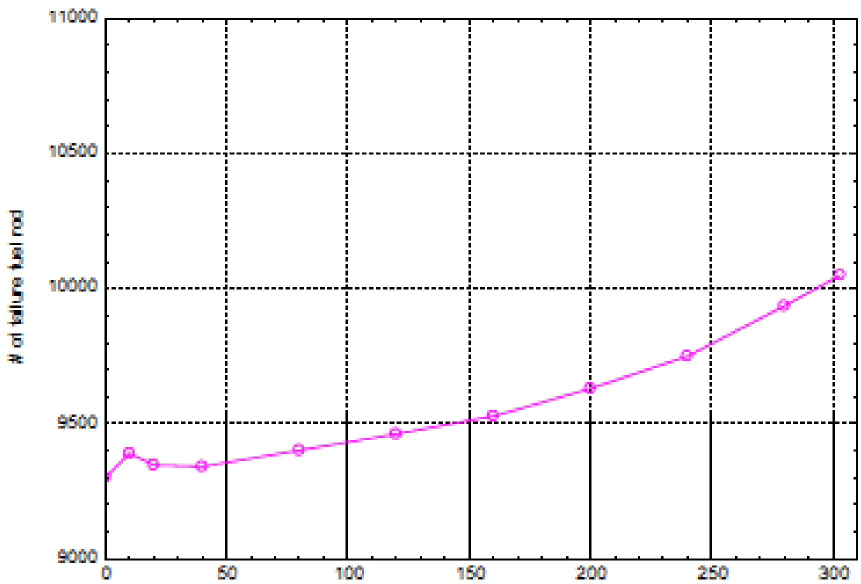

Figure 5: Number of failed fuel rods during cycle

- <u>Integral code coupling and 3D core modelling</u>
  Two partners developed this methodology with two different tools and calculation chains. One of these two concerned the development of the DRACCAR approach based on 3D eighth core model (**Figure 6**). During the project, the DRACCAR code was extended by introducing new burst criteria, improving 2D

core model. Case studies were used to discuss specific modelling points in DRACCAR with respect to LOCA phenomena - such as rod to rod interaction - or modelling scale - such as equivalent rod or pin-by-pin model. A whole calculation chain chaining DRACCAR with ASTEC FP modules dealing with FP transport and chemistry in primary circuit and containment was also built. In this way, the global methodology used during the project for PWR-900 radiological consequences evaluation of LOCA DBA and DEC-A transients was based on VESTA, FRAPCON, DRACCAR and ASTEC software [30]. The second partner developed an approach with full RPV and 3D core model with ATHLET-CD (**Figure 7**). Review of the available creep and burst model available in ATHLET-CD was also carried out. The approach was illustrated on Konvoi reactor for LB LOCA. Failed rod number was evaluated with 3D RPV model and burst rod location was found to be non-symmetrically distributed [30].

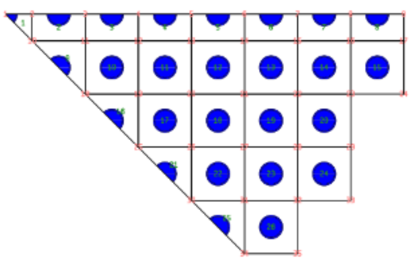

Figure 6: DRACCAR 3D modelling of 1/8th of PWR (26 FA) assuming symmetries

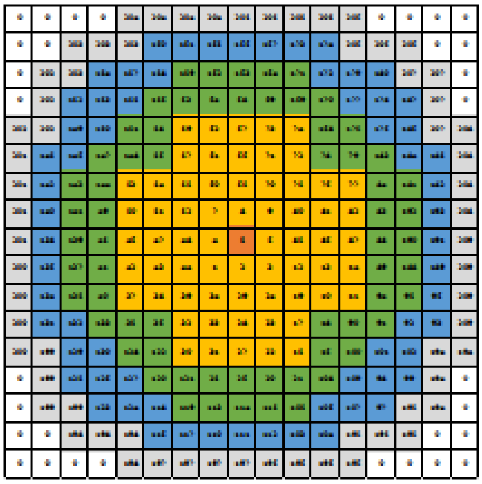

Figure 7: ATHLET-CD 3D core modelling (location of 196 FA and assignment to core ring)

Finally, in some cases, both approaches (BWR-4 LOCA DEC-A analyses) were used, the fuel performance code (TRANSURANUS) results being used to complement the calculation with the integral code and further refine its core nodalisation.

As illustrated above, used methodologies and core models differed widely between partners. Indeed, the modelling choices and the simulation approaches strongly vary with the choice of software and simulation chain. However, all approaches intend to describe as best as possible the different characteristics of fuel rods in the core. The most advanced 3D core models using integral codes seems to present benefits in comparison to other core descriptions as firstly the thermal hydraulics and the thermomechanics are coupled and secondly the resulting detailed core description can capture 3D effect associated to fuel assembly location or asymmetrical core cooling. However, one limitation of these 3D approaches remains the higher CPU cost which is not appropriate to run large number of simulations needed for instance to manage uncertainty analysis.

For all these different approaches, prospects were identified to further improve the simulation or the code capabilities and extend the predictive capacities associated to failed rod number evaluation.

4.3 Fission product transport and behaviour up to environment

The areas of interest of this work were very broad and comprised model improvements and/or validation in the following topics:

- Core inventory,
- Fission product release from the fuel rod,
- Fission product transport in the primary circuit,
- Fission product behaviour in the containment.

Regarding core inventory, activities were performed aiming at precise estimation of a VVER-1000 core inventory at fuel assembly scale, which is an essential part of the radiological consequence estimation and preceding fission product transport within the primary circuit and containment. In this study, the recalculation was done with SCALE code, using state of the art methods and best estimate approach to reduce the conservativism.

Regarding fission product release from the fuel rod, several activities were performed on various codes.
Some verification & validation of the models embedded in the ASTEC/ELSA module dealing with FP releases from fuel for the conditions of interest in the project (DBA & DEC-A) was performed. The work was focussed on volatile FP releases from high burn-up fuel for which increased volatile release is expected and for which there is no specific model in ELSA, causing some discrepancies in high burn-up validation cases (**Figure 8**) It was intended to, through optimisation of fuel grain size distribution, to reproduce artificially the effect of burn-up on FP releases. For the optimisation two VERCORS tests with two different burn-up were chosen : VERCORS RT1 and RT6 experiments (respectively 47.3 and 71.8 GWj/t) The optimisation study was performed using RAVEN tool coupled with ASTEC, performing 1000 calculations and selecting the distribution and range of 3 main parameters of the ELSA module (**Figure 9**).

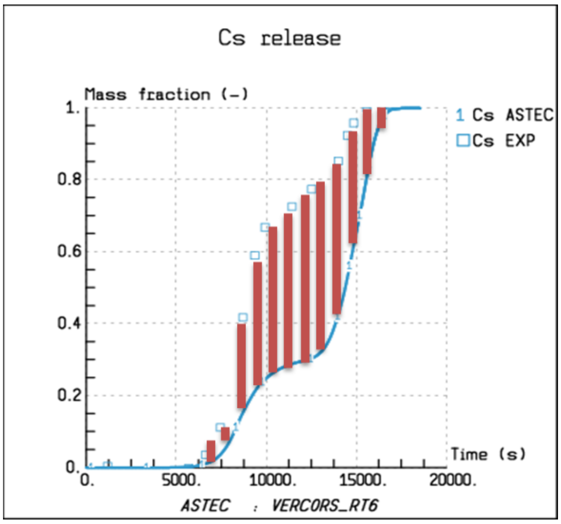

Figure 8: VERCORS RT6 Cs releases : experimental vs ASTEC/ELSA initial calculations

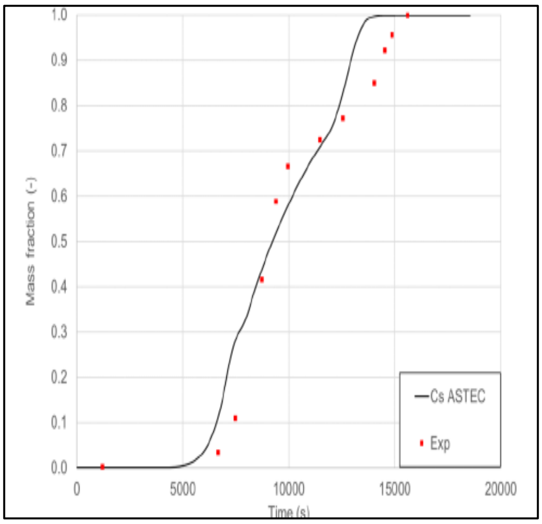

Figure 9: VERCORS RT6 Cs releases : experimental vs ASTEC/ELSA optimised calculations

A detailed analysis of fission product release from fuel during DBA LOCA conditions with ATHLET-CD code was also performed. The simulations were done on a German PWR Konvoi NPP model. The simulations revealed that due to the physical nature of the LOCA transient (especially DBA) majority of the fission product release originates from the fission products accumulated in the fuel-cladding gap. ATHLET-CD is equipped with three burst models, where two of them were found to have severe issues. At the end, the only fission release model applicable for DBA-LOCA was found to be the one based on CORSOR. From this analysis it was concluded that future effort is needed to precise estimation of the fuel-cladding gap inventory.

The models implemented in ASTEC-TR module SOPHAEROS for FP transport in the primary circuit and behaviour in the containment (incl. iodine chemistry) were re-assessed and their applicability to DBA and DEC-A condition verified. Indeed, these models were originally validated on several experiments (Phébus-PF, ISTP, OECD/STEM) aiming mainly at iodine behaviour but for initial and boundary conditions representative to DEC-B conditions (characterized by higher temperatures and dose rates). The comparisons revealed good agreement with experiments chosen from the R2CA database, either for transport in the primary circuit, or for transport and chemistry of iodine in the containment. The figure below illustrates the experiment-calculation comparison for time-dependant inorganic and organic iodine releases from Epoxy paint previously loaded with iodine and further irradiated in gas phase.

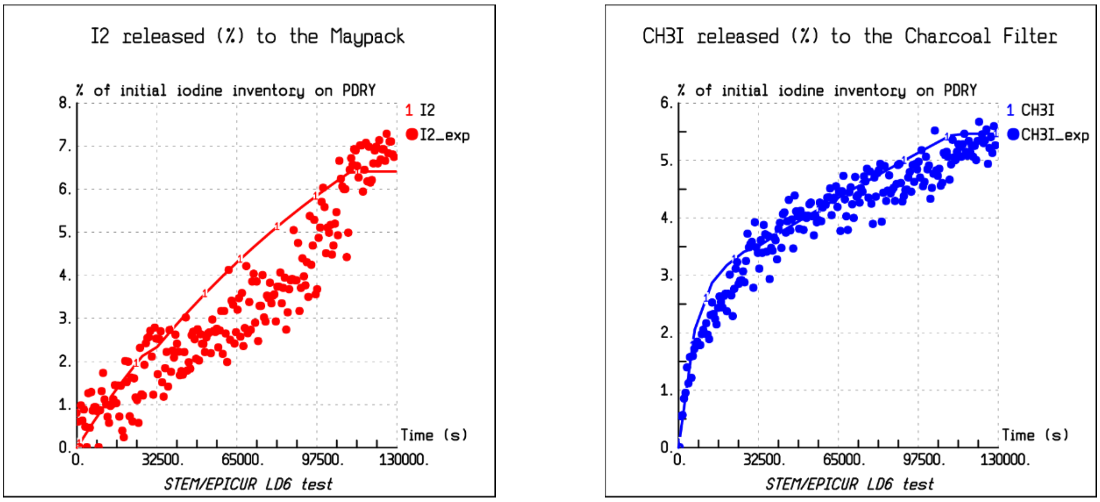

Figure 10. Inorganic and organic iodine releases from Epoxy paints irradiated in gas phase (EPICUR LD6 test): measurements vs ASTEC-TR calculation results

In addition, regarding iodine chemistry in the containment verification and validation of the models implemented in COCOSYS on several BIP experiments aiming at adsorption/desorption on dry painted surface were also performed. In particular the models were fine tuned to the Ameron Amerlock paint in VVER-1000. Further validation aimed at RTF experiment, where the impact of pH on iodine revolatilization was studied. The results were then transferred to the VVER-1000/V-320 containment model, where sensitivity studied aiming at sump pH proved the consonance with the RTF experiment. Finally, a BEPU analysis using the GRS methodology and Spearmann's correlation ratio marked important initial and boundary conditions (i.e., sump pH, spray droplet diameter, spraying angle, environment pressure) for the iodine releases in the containment, which was thoroughly investigated earlier (**Figure 11**).

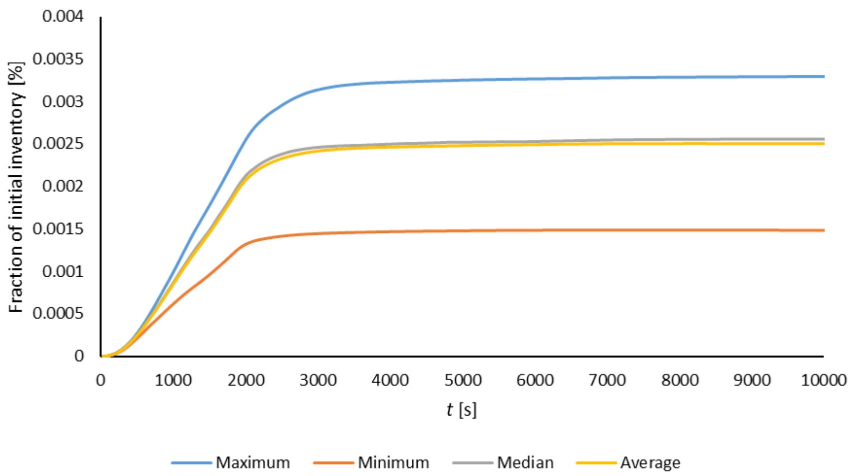

Figure 11 Results of the BEPU analysis of iodine release from VVER-1000/V-320 during LB LOCA (COCOSYS calculation)

Finally, some validation work was performed for a newly aerosol gravitational deposition model implemented in APROS code. The model was satisfactorily compared to both MELCOR calculation results and AHMED experimental data.

The main goal of the project, reduction of uncertainties, was the linking element of all the activities conducted by the partners in this work. The expectations were fulfilled. Furthermore, several areas for future development have been targeted. The main issue is the validation, where many of the implemented models were validated against conditions, which are typical to DEC-B (high temperature, high pressure, high dose rate etc.) and a proper validation on DBA and DEC-A conditions should be conducted. Future effort should be aimed at precise definition of typical LOCA conditions (for fuel, primary circuit, and containment). Based on that, a complex reassessment of existing experiments should be done to select relevant experiments for validation and to reveal knowledge gaps, i.e. missing data and conditions. These gaps may become corner stones of future research projects both in national and international level. As mentioned earlier in this report, the need of research of the DBA and DEC-A conditions is even more important for SMRs (small modular reactors), where the DEC-B conditions are expected to be practically eliminated due to inherent safety.

5 Main Progresses in SGTR modelling

For SGTR transients in DBA and DEC-A the phenomena of interest and associated issues that have been considered during the project in support of more realistic evaluations of their radiological consequences include the behaviour of FP during their transfer from the primary to secondary circuit (incl. complex coupled phenomena of thermal-hydraulics, physics and chemistry of gases and aerosols), the primary circuit contamination due to the presence of defective fuel rods, potentially rapidly increasing during the transient (dealing with the FP releases from fuel to gap but above all with the escape of FP from defective fuel rod gap to primary coolant). Modelling the defect occurrence in a fuel rod was clearly out of the scope of the project and for all the SGTR calculations performed the primary circuit contamination prior to the transient was issued from NPP measurements or assimilated to the current maximum technical specifications. Furthermore, the project also deserved a specific attention and dedicated work on the secondary hydriding of defective fuel rod inner clad in normal operation conditions, as this phenomenon can potentially lead to a subsequent clad failure during a SGTR transient and fuel fragment dissemination in the primary circuit. The models developed on this topic were however not applied in reactor calculations.

Different approaches can be used to evaluate the source term for this type of accident, where a good prediction of the primary circuit contamination and of the FP distribution/evolution in the failed SG is crucial if we are to assess their consequences more realistically.
The main model improvements carried out during the project focused on the primary circuit source term (i.e., gap FP inventory and FP releases from the defective fuel rod), the FP transport in the primary circuit (dilution…), the FP transfer from the primary to secondary circuit (incl. flashing, atomisation, scrubbing, partitioning…) and the clad secondary hydriding.

5.1 Secondary clad hydriding

As mentioned earlier, the weakening of defective fuel rod clad due to its internal secondary hydriding can potentially lead to clad rupture and fuel dissemination in the primary coolant. As a matter of fact, though the modelling of this additional source term in the primary circuit was beyond the scope of the project, a great attention was paid during the project in modelling the clad secondary hydriding and exploring the resulting risk of defective fuel rod failures due to cladding ductility evolution. Such a phenomenon has been a major issue for BWRs in the last 80s where following secondary defect appearances, significant degradations of defective fuel rod clads were observed, mostly consisted in hydrides blisters or axial cracks, and in the most severe cases in extended fractures.
Many causes and phenomena can lead to fuel cladding damage during reactor operations, such as stress corrosion cracking, grid-to-rod fretting, debris induced failure, among others. Over the years, with improved knowledge and best practices for fuel fabrication and design, the probability of fuel failure has however been reduced to low levels. For the Pressurized Water Reactors (PWR), the worldwide fuel rod defect rate between 2006 and 2015 was typically around 0.004% (IAEA, 2019). Nevertheless, even with such low a defect probability of occurrence, understanding and better modelling the behaviour of defective fuel rods, especially its clad weakening/failure through secondary hydriding, remains of significant importance, due to its potential great impact on the environmental radiological source term in SGTR scenarios where the containment is by-passed.
Activities on this topic within the project were restricted on the phenomena of secondary hydriding of Zr-based alloy claddings within normal operation conditions (i.e. 300-400°C). They involved both experimental and modelling activities.

<u>Experimental work</u>: Hydrogen uptake tests have been carried out E110G and Zircaloy-4 cladding tube samples between 300 and 400 °C [31]. Text matrix covered four different temperatures for each alloy and each test includes four ring samples. H_2 uptake was calculated both from the H_2 pressure decrease and mass gain. Differences in H_2 uptake between E110G and Zr-4 were evidenced as well as in its temperature dependence (**Figure 12**). For both clad materials, an increase of H_2 uptake with temperature was measured. The detailed information included in the R2CA database further allowed to improve numerical models on the H uptake process.

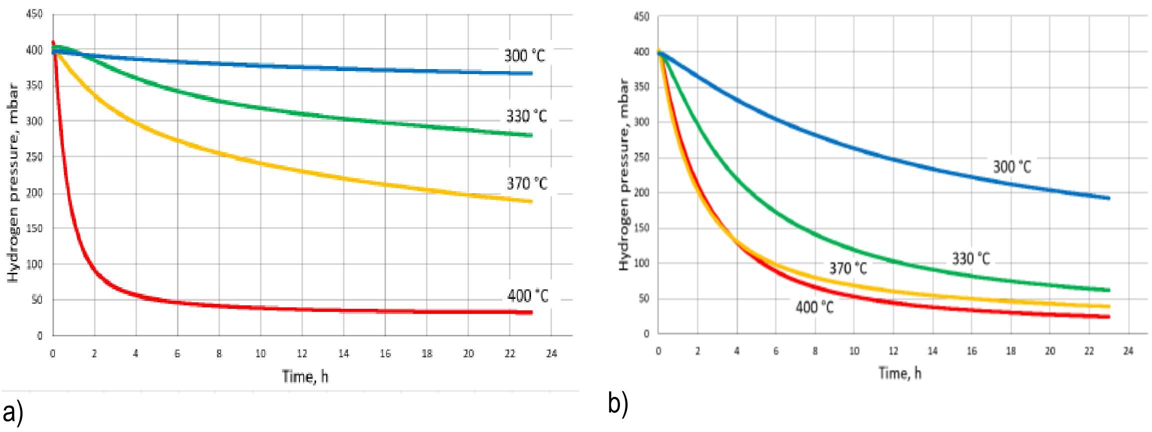

Figure 12: H_2 uptake experiments on E110G (a) and Zr-4 (b) samples: H_2 pressure evolution at different temperatures

<u>Modelling activities</u>:
First a simple exponential correlation (driven by H_2 partial pressure and temperature) dedicated to H_2 uptake was developed based on the experimental results above mentioned for temperature and H_2 partial pressure ranging respectively from (300-400°C and 0-400 mbar). Experimental results were found to be satisfactorily reproduced by the model at lower temperatures and higher pressures while at higher temperatures the calculated H_2 uptake became overestimated at lower pressures. Based on the new experimental data obtained regarding the H2-uptake model a critical assessment of the model embedded in TRANSURANUS code for LOCA conditions was also carried out indicating that the extrapolation of the modelling parameters in much lower temperature ranges does not allow obtaining reliable results and would necessitate for this temperature range to re-evaluate the model parameters for the gas-solubility together with the activation energy.

Besides several development/enhancements of models were performed further embedded or coupled in/with detailed codes (fuel performance codes such as TRANSURANUS, FRAPCON or dedicated one such as SHOWBIZ) aiming at considering the whole secondary hydriding phenomema occuring in a defective fuel rod from water ingress to hydride blister formation. At the project onset indeed none of the simulation tools used in the project were able to simulate the whole phenomena in normal operation conditions. Depending on the codes, these models were related to internal gas transport in fuel rod free volumes, clad internal oxidation, clad H_2 uptake, H_2 redistribution in the cladding and/or hydride precipitation/dissolution.
In particular different models were derived for the H_2 redistribution within the cladding which is the key phenomena for the formation of a secondary defect (blister). That was the case for TRANSURANUS and for the external model coupled to FRAPCON. This latter was adapted during the project by including a new modelling for H_2 precipitation/dissolution derived from the Hydrides Nucleation-Growth-Dissolution model [32]. In this new model the hydride precipitation includes nucleation of new hydrides and growth of existing ones and a kinetic constant for hydride dissolution is taken into account. This new model together with alternative solid solubility limits was shown to be able to reproduce more adequately the data from an experiment that consisted of a series of thermal transients applied to an H_2-loaded sample [33], where successive dissolution and precipitation of hydrides were induced (**Figure 13**).

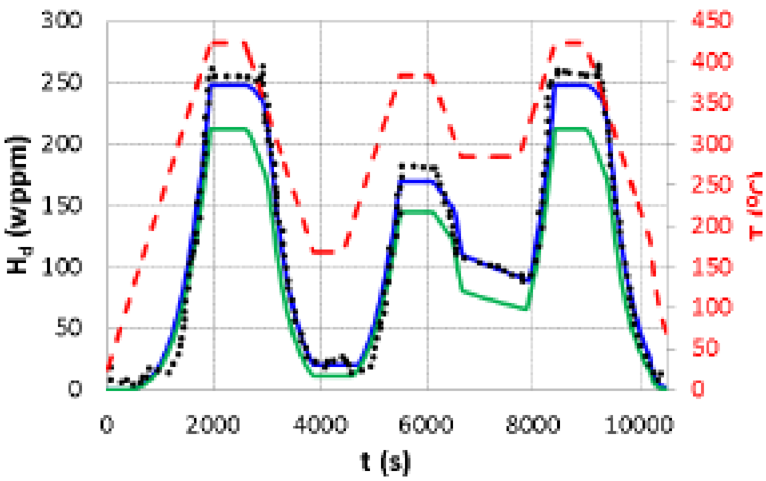

Figure 13: Dissolved hydrogen evolution against experimental temperature evolution (red): measured (black) vs calculated using two different solid solubility limits for dissolution & precipitation (defaults one in green, updated ones in blue)

Applied to study the H_2 distribution after a massive hydriding in a Zr-4 clad of a defective fuel rod at the beginning of life coupling, the updated model (slowing down the H_2 adsorbed distribution across the cladding thickness and giving rise to localized accumulation of hydrides) highlighted the importance to properly simulate the hydride precipitation/dissolution phenomena for an adequate prediction of the in-clad hydride distribution (**Figure 14**).

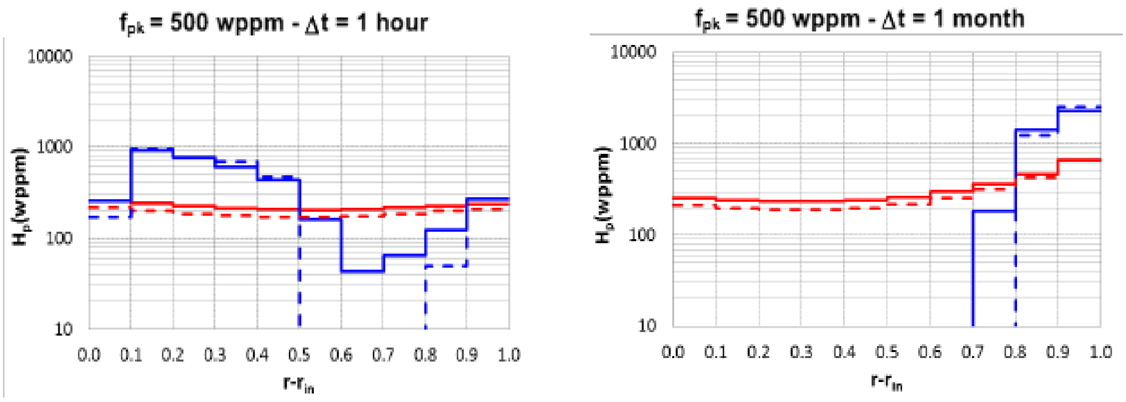

Figure 14: Precipitated H_2 distribution across the cladding thickness at 2 different times after massive hydriding. Comparison of the initial (red) with the new modelling (blue) using different solid solubility limits: default ones (continuous lines) and updated ones (dashed lines)

More complete simulations of key phenonemena occurring in a defective fuel rod have been performed with the dedicated tool SHOWBIZ. It included both a 1-D channel modelling (with clad internal oxidation, and H_2 uptake, internal redistribution of the gaseous species in fuel rod free volumes (gap & fuel porosity) coupled with a 2-D cladding modelling (with internal H_2 diffusion, dissolution/precipitation and blister formation). The results indicated the formation of a secondary blister defect at the external side of the cladding one month after the occurrence of the primary clad defect (**Figure 15**). The position of this secondary defect with respect to the primary one was found to be in accordance with French NPP feedback.

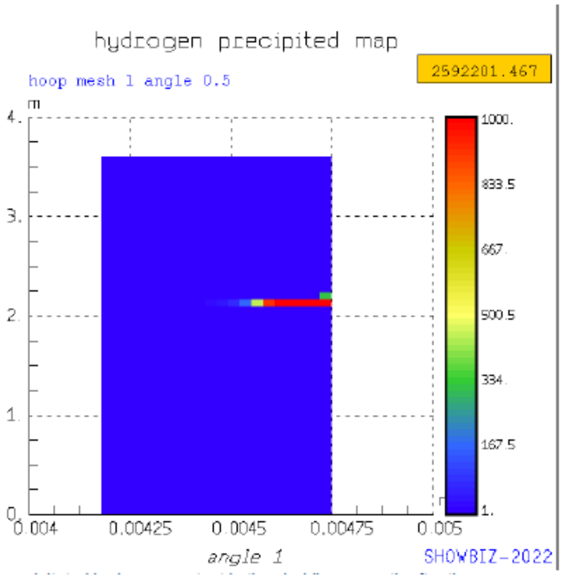

Figure 15: 2D map of H_2 precipitated content through a Zr-4 cladding one month after the occurrence of a primary clad defect locating 30 cm from the fuel rod bottom

5.2 Primary circuit source term

Activities were devoted to improving models and tools to describe the behaviour of defective rods during SGTR transients, mainly the release of gaseous and volatile fission products (FPs) and the fuel oxidation.

<u>Primary source term evaluation: fuel-to-gap release</u>

As for the modelling of the radioactive release from the fuel to the gap, a methodology to bound a priori the numerical error on the prediction of radioactive FP/gas release with SCIANTIX was developed [34]. The methodology was tailored to state-of-the-art SDAs and aimed to determine the number of time-steps of modes used in the computation of the numerical solution. The methodology is applicable both in constant and transient conditions, it is suitable for implementation in simulation codes of interest for the current task and to reproduce reactor conditions pivotal for the project. A physics-based model was also developed to describe the intra-/inter granular behaviour of radioactive FG/FP in the fuel, to reproduce the dynamics of the radioactive release and its evolution during irradiation [5]. This development constituted a milestone in the modelling of radioactive gas without calibration of specific parameters, as in the ANS 5.4-2010 methodology [35], under both constant and transient conditions. The model has been implemented in SCIANTIX and tested as a standalone code against the CONTACT1 irradiation experiment, from the IFPE database [5, 36, 37]. Results included the comparison of the release-to-birth ratio of several short-lived isotopes of xenon and krypton with both the experimental measurements and the predictions given by the semi-empirical ANS 5.4-2010 methodology. In order to assess the aforementioned model from an integral point of view, the coupling interface between the integral fuel performance code TRANSURANUS and SCIANTIX has been upgraded, to account for the TRANSURANUS restart option. Then, the coupled code TRANSURANUS//SCIANTIX has been used to reproduce the CONTACT1 and the HATAC C2 irradiation experiment. Results shown in **Figure 16** for the simulation of the CONTACT1 CASE revealed the potential of the coupled version of TRANSURANUS with SCIANTIX [38].

Meanwhile, the implementation of the semi-empirical model ANS 5.4-2010 by V. Peri was reprogrammed in modern Fortran in the TRANSURANUS code to predict the release-to-birth-ratio of some short-lived gaseous and volatile FPs. TRANSURANUS code calculations were also used to refine the conservative assumptions regarding the number of the failed rod in the core at the initiation of the SGTR. The gap inventory of ^{135}Xe, ^{133}Xe, ^{131}I and ^{137}Cs were assessed by TRANSURANUS model for both an intact fuel rod and a fuel rod with an assumed prior cladding breach. The calculated gap inventories were compared to the coolant activities measured in a VVER-1000 plant. Several cycles with varying number of leaking fuel rods were analysed. No clear conclusion could be made for the release rates during the normal operation, including small activity spikes following power changes. On the other hand, the shutdown spike activity of ^{137}Cs was found to always corresponds well to the gap inventory of the leaking rods assuming no enhanced diffusion from the fuel as a result of the cladding failure. This conclusion helps to justify the application of the TRANSURANUS code for the gap inventory analysis.

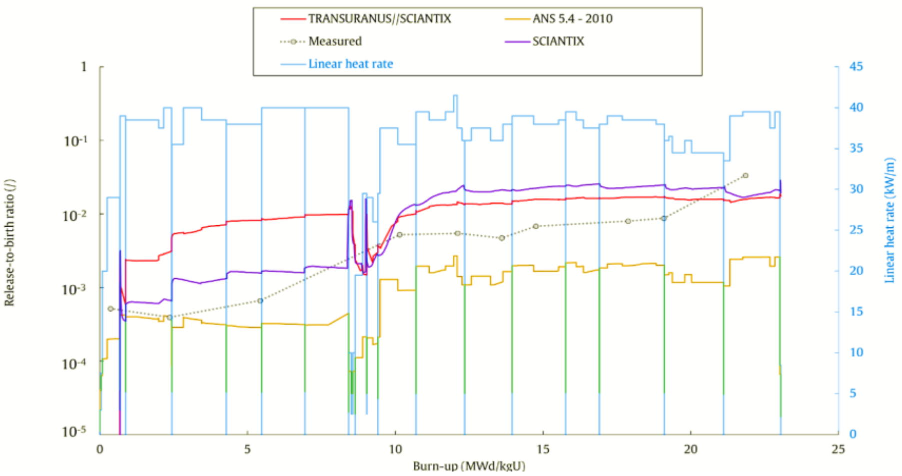

Figure 16: Release-to-birth ratio of Kr-85M as a function of fuel burn-up: CONTACT1 experimental data vs calculations

The TRANSURANUS code itself was further upgraded with a specific model for radioactive FP release from defective fuel rods [20]. This model was structured in two successive steps: (1) FP release from the fuel to the fuel-cladding gap and (2) FP release from the fuel-cladding gap to the coolant. Results for the release from the fuel to the fuel-cladding gap have been compared with experimental data for CONTACT1 experiment of the IFPE database. As for the release from the gap to the coolant in case of defective cladding, the model exploited a phenomenological first-order rate theory description to estimate escape rate constants under equilibrium conditions, and results have been compared during the simulation of the CRUSIFON1bis experiments (**Figure 17**).

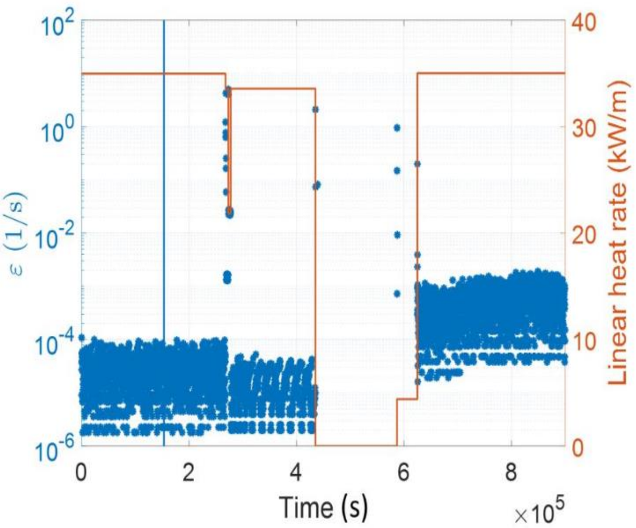

Figure 17: Experimental time-dependant escape rate coefficients of Xe-133 from defective clad to primary coolant in CRUSIFON1bis (vertical blue line at 170000 s is time at which steady-state conditions were reached)

Finally, a new methodology using the coupled TRANSURANUS and MFPR-F codes for evaluating the release of radioactive isotopes from the fuel was developed. It was based on a decoupling approach treating separately the release problem of (stable) elements, and the decay/release problem of radioactive isotopes. This approach allowed to perform accurate assessment of the element release (incl. FP chemical interactions and fuel oxidation by the gap atmosphere strongly affecting the FP releases such as I and Cs) and to reuse this assessment for the calculation of radioactive isotope releases. The decoupling approach used two separate tools: the coupling of TRANSURANUS and MFPR-F codes, and a simple calculation tool for the formation, decay, transmutation and transfer of radioactive isotopes. The use of this latter tool considering only Booth diffusion releases requires a preliminary fitting of its parameters based on TRANSURANUS/MFPR-F results which simulated more complex release mechanisms more suitable for FP like iodine. This approach has been applied to an irradiation case taken from the Halden database (IFA-650.10) simulating a cladding defect to illustrate the differences in release-to-birth ratios evolution of FG and iodine isotopes.

Primary source term evaluation: gap-to-coolant release

The open literature about f fission product release from defective fuel rods under primary to secondary leaks (SGTR transients) was reviewed (related to the “spike” phenomena) by different partners. It was noticed that data concerning iodine spiking came mostly from western-type Pressurized Water Reactors (PWRs) such as they were operated more than 3 decades ago. Thus, also valuable for developing models, their direct applicability might be questionable for the currently running fleet, which uses different fuels under different chemical conditions of the reactor coolant system and conditions of operation, and for which also clad defect occurrence is expected to be lower.

At the onset of the project only few models were available for iodine spiking in the analytical tools used and often conservative approaches were used based on guidelines like [40, 41], in which the release rate estimated during steady state is assumed to increase 500 times for 8 h. In some cases, NPP data were used where often only peak values are available. That is why great attention was paid during the project on investigating approaches for iodine spike-effect modelling. In particular, to compare the actual VVER-1000 spike events versus the approach specified in NUREG-0800 [39] and regulatory guide RG 1.183, information on the spike events at NPPs with VVER-1000 reactor operating in Ukraine for last 10 years were collected and analyzed (this information could be submitted by Ukrainian Utility NNEG Energoatom only with request). It was unfortunately concluded that the scope of data available is insufficient considering that reported data provides the peak values for the iodine activity only with no information on activity change with time, and do not include information on actual purification system performance during the spike event, which is needed to estimate the total iodine removal rate. Therefore, the applicability of NUREG-0800 and RG 1.183 approach for estimating the iodine spike for VVER-1000 nuclear fuel could not be performed based on the currently available data.
Concerning the modelling of iodine spiking, further developments were carried out in the RING code against new 18 nuclear power plants data (during power transients, reactor shutdown and start-up). The targeted developments have been oriented to overcome limitations in previous version of the code, and the introduction of new caesium spiking models (^{134}Cs and ^{137}Cs). The upgraded RING code was applied to the simulation of iodine and caesium spiking effect in SGTR, and collector cover opening conditions. It allowed to precise the activity release according to the specific power and pressure histories of the two events. In the updated transient model of the RING code, the release accelerates as a function of the variation in core power, primary pressure, and boric acid concentration. Results for calculated activity release and core inventory of ^{131}I, ^{134}Cs and ^{137}Cs isotopes during two different SGTR events (break of 3 tubes and collector cover opening) are shown in **Figure 18**.

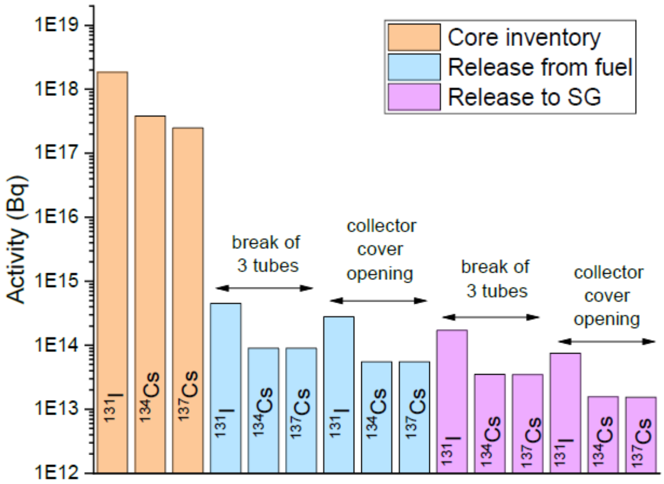

Figure 18: I131, Cs134 & 137 core inventory and activity releases from fuel and to SG during SGTR events calculated with the upgraded RING code

Meanwhile, the capability of RELAP5-3D to simulate iodine behavior during a SGTR scenario was also analyzed. It was concluded that the built-in model of the code was not sufficient to simulate the chemical transformation of FPs adequately. Therefore, an external empirical function was developed to improve the FP behaviour during the transient simulation, in which, in addition to reactor power as in the previous model [39] the time point in the fuel cycle was considered. The model was based on an extensive review of the data regarding the fuel cycle and primary circuit contamination of the different reactors in the US nuclear fuel annual reports.
Finally, as for iodine spiking and severe accident codes (i.e. MAAP5 and MELCOR) different approaches were used to improve their modelling. In MAAP5 a simple iodine spike model easily controlled by the code user was implemented including multiplicative factors for iodine, caesium and the rest of FPs. In MELCOR, where the models not applicable for SGTR events initially predicted no FP releases for fuel temperatures lower than 900°C, ad-*hoc* user functions were developed to estimate less conservative iodine releases from failed fuel rods. Based on [42],

they simulate the release rate of iodine considering the enhanced-diffusional release during reactor shutdown and includes any forced-convective release that may occur because of the temperature and pressure changes during the shutdown event.

5.3 FP transfer from primary to secondary circuit

The release of fission products, particularly iodine, and their transport into the secondary side of a failed steam generator in case of a DBA/DEC-A SGTR sequence, were considered areas where further enhancements might have a sizeable impact when simulating the radiological consequences of such scenarios. To do so, first a thorough review of the available data was performed. Specific data addressing phenomena potentially occurring during the transfer of fission products from primary-to-secondary circuit, like flashing, atomization and partition were found hardly available (in THAI [42], ARTIST [44, 45] experimental programs, US SGTR accident investigation program [46], particularly under the prevailing conditions in the scenarios addressed.
However, based on the insights gained a variety of new models and/or approaches have resulted.
At the project onset, practically no specific models for the transport into the secondary side of the failed steam generator were available, except in the case of the MELCOR code, which does have some modules that might be used for the purpose.

The models enhanced in R2CA can be grouped according to the nature of the code used:

- Thermal-hydraulic codes, like RELAP5 3D, have extended their abilities regarding fission product transport. Two different approaches have been adopted. One is based on the boron tracing model existing in RELAP5. The other is based in post-processing the thermal-hydraulic variables from the code an applying decontamination factors to account for processes such as purification in the primary circuit or scrubbing in the secondary circuit (**Figure 19**). More details regarding these two approaches can be found in [47, 48].

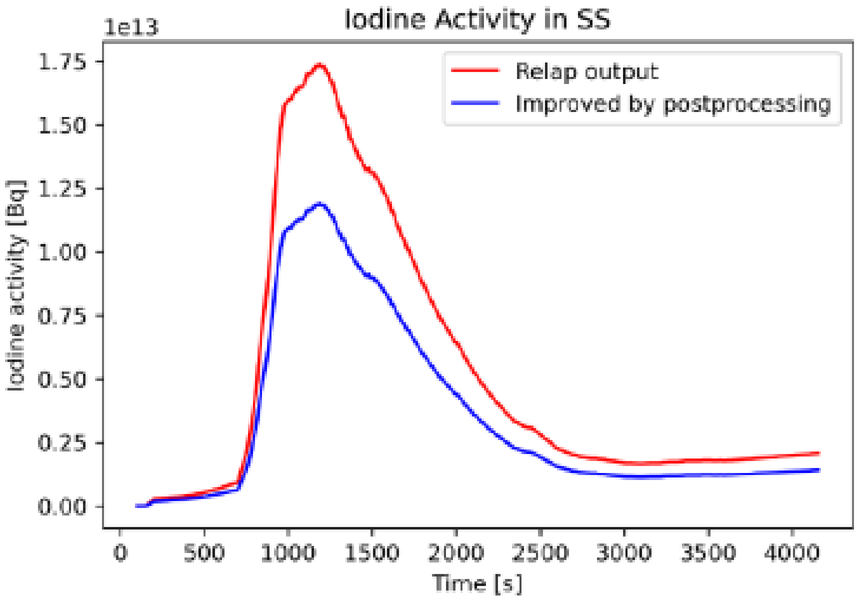

Figure 19: RELAP5-3D calculations: effect of pool-scrubbing on iodine concentration in SG secondary circuit

- Severe accident codes, though, show a variety of approaches that were developed within the project. ASTEC was enabled by two additional modules dealing with mechanical fragmentation and flashing of the primary water jet and radioactive transfer from the primary to the secondary circuit and, eventually, to the environment (DROPLET and SAFARI, respectively), which details can also be followed in [48]; MAAP5 was extended with optimized primary-to-secondary transport correlations [48]; and finally MELCOR was activated using in-code thermal-hydraulic capabilities for water discharges under high pressure differences and applying the partitioning of molecular iodine through user-defined functions [48].

6 Re-assessments of LOCA Radiological Consequences

The same scenarios as calculated at the project start were recalculated with the improved simulation tools and calculations chains. The benefits due to improvements, from core to environmental FP release modelling, were analysed and highlighted through the environmental source term and radiological consequences evaluation.
The 2nd set of LOCA calculations mainly benefited from three types of improvements (detailed in the previous sections):

1. The code modelling: i.e. use of more appropriate thermomechanical models for clad ballooning and burst, of new clad burst criteria…,
2. The core models: i.e. use of more detailed 3D T/H core models, or core models updated based on results from parametric analyses or from more detailed (mechanistic) fuel performance code …,
3. The calculation chains: i.e. use of detailed (mechanistic) fuel performance codes not only as a support of less-detailed tools, but also as an integral part of the chain for a better coupling of thermohydraulic and thermomechanical models at the subchannel level; use of new simulation tools in the chain….

Main model improvements made were related to fuel rod burst. For VVER this involves the use of thermomechanical models instead of the very conservative assumptions if all fuel rods would fail during the transient. For Konvoi also the 10% failed rod ratio for DBA issued from regulatory practices were replaced by thermomechanical calculations of fuel clad behaviour and updated core modelling. For PWR-900, improvements of both clad burst models/criteria and core modelling were provided. For EPR, in addition, new cladding creep and phase transformation laws for M5 clad materials were used for updated DBA calculations. Finally, some partners, by using new tools in their calculation chains, improved their core modelling or the modelling of FP releases from fuel and transport up to containment.
Thanks to this, the number of burst fuel rods in the core was generally reduced for all reactor concepts for DBA and DEC-A transients (especially for VVERs). Exceptions were for EPR in DBA where a more stringent clad failure criteria was used and for PWR-900 DEC-A due to a more detailed 3D core modelling. As there have been no changes in thermal hydraulics nor major modifications in the modelling of FP transfer in primary circuit (except for Konvoi) and containment vessel, the changes in burst fuel rod ratios directly influenced the activity releases in the environment. That is why significant differences in environmental activities between the two sets of calculations were observed for VVER. In the end, the relative reduction in environmental activity releases was ranging from 80 to 100% for all NPP concepts for DBA transients (**Figure 20**) and form about 13% to 99 % for DEC-A (**Figure 21**).
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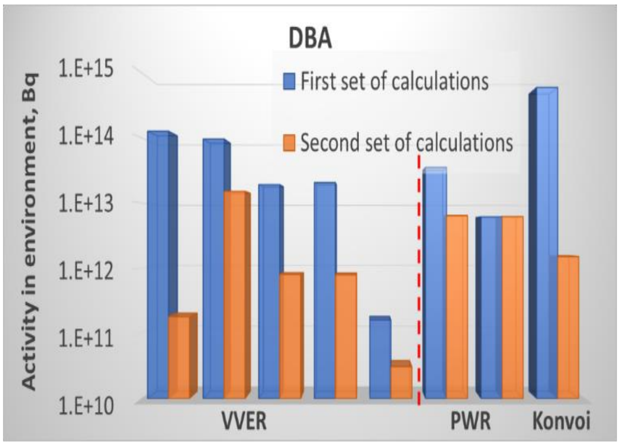

Figure 20: Activity releases in LOCA DBA

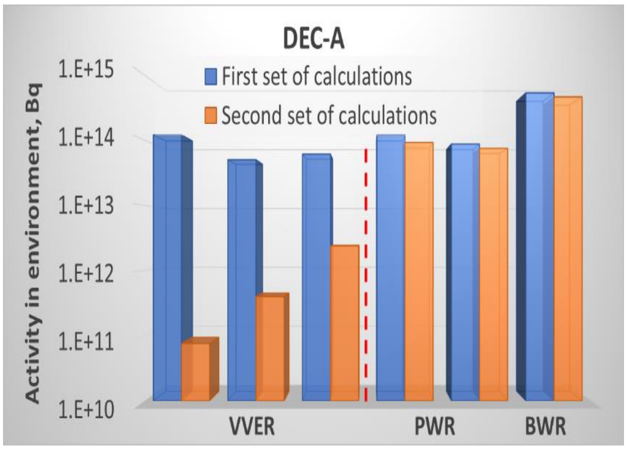

Figure 21: Activity releases in LOCA DEC-A

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The discrepancy between all the results was reduced for DBA calculations but increased for DEC-A. Several reasons can explain the remaining discrepancies in updated calculations for which conservatisms and decoupled approaches have been reduced such as differences still in initial/boundary conditions, modelling and NPP operation in LOCA… (i.e. gap inventory, design containment leakages, CSS operation and efficiency, and for iodine (differences in iodine form fraction, consideration of iodine chemistry or not), list of isotopes considered…).
Additionally, several methodologies using different modelling computer codes or process assessment methods were applied by the partners that are also impacting the results. For example, for the core modelling itself two different methodologies were used:

- Some partners used thermohydraulic codes chained to a fuel performance code. In this case, the core and the reactor core system are simulated given a chosen scenario and assumptions and results in terms of thermohydraulics are used as boundaries conditions by the fuel performance code.
- Other partners used an integral approach with codes (generally Severe Accidents codes) dealing with RCS, thermalhydraulics and fuel thermos-mechanical modelling in the same simulation. In this approach the core thermohydraulics and thermomechanics are strongly coupled.

Evaluated radiological consequences (thyroid equivalent and total effective doses) were consistent with what is observed with the activity calculated in the environment: for most calculations, especially for VVER, radiological consequences were reduced in the second set of calculations compared to the first one. The calculated doses for all LOCA transient conditions (DBA and DEC-A) stayed under acceptance criteria.

The more detailed calculations performed within the project showed a strong dependance on gap inventory/source term, rod internal pressure, rod power distribution, local variations of cooling implying the needs for a better estimation of fuel axial gas transport, fuel assembly characteristics (burn-up, location…) and a whole 3D T/H core modelling. This latter when used in some of the updated calculations significantly strongly increased the CPU time. In some cases, even, limits of the modeling tools were achieved, and it was necessary to find a compromise between needed details vs computational effort. This challenging problem was not solved in the frame of the project, however possible solutions have been suggested (i.e. computational time reduction methods, specific calculation methodologies mixing very detailed and less detailed modelling of the core…).
Though the calculation schemes and modelling were greatly improved during the project, some limitations have been identified where further improvements would be still needed for best-estimate evaluations (i.e. considering fission product multi-gap inventory, increasing the number of equivalent fuel rods & associated T/H channels, reducing CPU of 3D T/H resolution…). Uncertainty analyses were also recommended to further improve the robustness of the developed methodologies.

7 Re-assessments of SGTR Radiological Consequences

The same scenarios as calculated at the project start were recalculated with the improved simulation tools and calculations chains. The benefits due to improvements, from core to environmental FP release modelling, were analysed and highlighted through the environmental source term and radiological consequences evaluation.
For the 2nd set of calculations, the improvements made for SGTR transient calculations were of two kinds:

- Modelling improvements: Partners dedicated improvements on the fission product modelling: initial primary contamination and spiking, dilution in RCS, transport, scrubbing, partitioning, atomisation, speciation etc. Partners also improved their thermohydraulic model using refined model for the relief/safety valves of the SG or by applying enhanced EOP.
- Improvements in the calculation chains: Detailed (mechanistic) computer codes were involved in the partners calculation chain as a support of less detailed codes for most of the part. For SGTR transient calculations, detailed codes were used for spiking, FP transport and dilution thanks to CVCS operation. Some of the partners used different modelling approaches comparing to what was used in the first set of the calculations.

As such, for SGTR scenarios, partners improved their simulation scheme mainly on the FP inventory and transport aspects. Therefore, except for two partners who also improved their thermohydraulic part as well, there is no change on the calculated cumulative steam/liquid water released in environment. Thanks to more realistic models for FP transport and interaction in the RCS and SG, partners achieved a reduction of the activity releases in the environment between 17 to 97 % (**Figure 22**, **Figure 23**). Nonetheless, two partners calculated higher activity releases with the second set of calculations. These results for these two partners can be explained by the consideration of new radioisotopes, FP speciation or releases in liquid phase which were not considered in 1st set of calculations. Overall, all partners improved their simulation scheme in order to provide more realistic results.

Evaluated radiological consequences were consistent with what was observed with the activity releases to the environment: radiological consequences were reduced in the second set of calculations compared to the first one, except for two SGTR transients. The calculated doses for all SGTR transient conditions (DBA and DEC-A) always stayed under acceptance criteria.

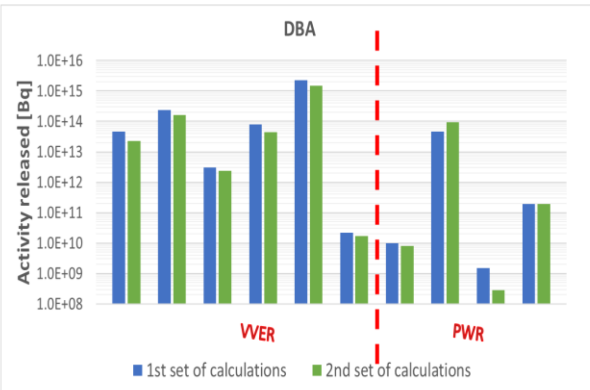

Figure 22: Activity releases in SGTR DBA

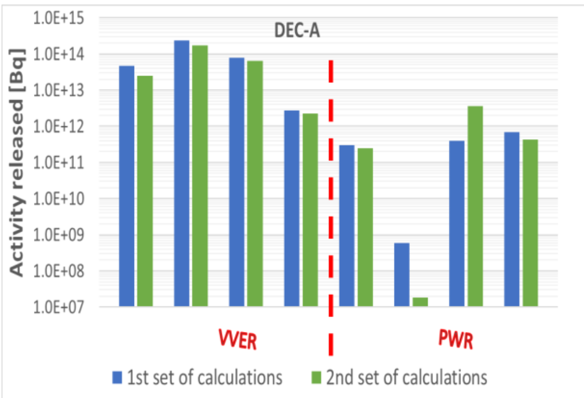

Figure 23: Activity releases in SGTR DEC-A

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However, it was still observed a large discrepancy between the results (up to 5 orders of magnitude difference between minimum and maximum activity releases calculated). Differences observed in the primary to secondary and secondary to environment discharges could be explained mainly by the differences in the scenario, the SGTR break sizes, the IS duration, automatic procedures and operator actions, in the secondary to environment

discharge capacities (SG relief and safety valves discharge capacities, setpoints, failures, operator actions, etc.) and in the considered initial and boundary conditions (additional single/multiple failure(s), best estimate/penalized parameters). These differences may also impact the evolution of the pressure in the RCS and in the affected SG that will further influence the water and steam released. Regarding FP and radioisotopes behavior, discrepancies between partners can also be explained by several reasons: differences on the initial FP inventory and spiking, differences on the isotopes considered, differences on the dilution in the RCS, differences on the transport phenomena through the SGTR break and in the SG (atomization, flashing, partitioning, scrubbing), differences in the consideration of activity releases in the steam phase only or in both liquid and steam phases etc..

Additionally, several methodologies using different modelling computer codes or process assessment methods were applied by the partners that are also impacting the results:

- Some partners used thermohydraulic codes which tend to be more faithful to simulate TH transient compared to integral SA codes. To simulate FP transport and behavior in RCS and SG:
    - Some partners used in-house conservative and simplified methodologies leading generally to conservative results in the 1st set of calculations. In the 2nd set of calculations, they tried to reduce the conservatisms considering different phenomena or by using modules embedded in their TH simulation code to simulate FP transport and behavior.
    - Other partners used specific and dedicated codes for radionuclides transport.
    - While other partners directly used modules and capabilities of their TH simulation code to simulate FP transport and behavior.
- Other partners used integral Severe Accidents codes to simulate at the same time TH and FP transport and behavior.
    - Some partners in this case had to developed dedicated in-house methodologies in order to simulate specific FP transport phenomena (atomization, partitioning, flashing for instance) as the SA code was not able to reproduce those phenomena because the code is not designed for that.
    - Other partners directly used the capabilities of their integral SA codes to simulate radionuclides transport and behavior.

Though the calculation schemes and modelling were greatly improved during the project, some limitations have been identified where further improvements are still needed for best-estimate evaluations:

- Retention and deposition of FP/radionuclides in the RCS/SG (in the swirl-vane or chevron separators for instance) should further be looked at.
- The radiological consequences of activity releases with liquid water phase should be better described so that they can be fully and independently considered.
- Uncertainty analyses are needed to further improve the robustness of the developed methodologies.
- For instance, the development of a mechanistic code which can simulate the FP spiking phenomenon based on gap inventory, burnup, fuel history (these data may come from specific mechanistic codes) and feedback from TH code (SCRAM and pressure transient) may be an improvement but one has to be careful on the ratios between improvement of the spiking modelling, CPU time consumption and added value of a more accurate spiking model compared to more simplistic model.

8 Recommendations towards a harmonisation of RC evaluation methodologies

A large amount of reactor calculations was provided during the project LOCA/SGTR DAB and DEC-A transients together with proposed improvements for more realistically calculating their environment radiological source term and then their radiological consequences. Quantitatively, an important dispersion appeared in terms of releases values (orders of magnitude) in both sets of calculations. This is the result of several factors like the hardware (PWR, VVER, BWR), the used calculation tools and methodologies, the duration of the release period considered, the list of isotopes and selected improvements between the 2 sets of calculations. Despite these differences between them, these calculations can be far from rough conservative evaluation and therefore contribute to a better estimation of the safety margins. From the comparison between the two sets of calculations (initial and improved) as well as from sensitivity analyses and uncertainty quantification carried out within the project the following recommendations for more realistically predictions have been formulated respectively for the two kinds of scenarios:

For LOCA transients

- Better prediction of failed fuel rods in a core is of first importance. To do so, expressing specific fuel rod initial conditions (i.e., burn-up, internal rod pressure, specific power, etc…) for thermos-mechanic calculations (incl. axial gas communication) and use refined criteria of cladding burst temperature and strain, specific to DBA and DEC-A conditions is important.
- To have a coupling between T/H and thermomechanical calculations. To this end, the use of a detailed 3D core modelling allowing for better differentiation of FA characteristics (power distribution) could be beneficial. It also allows to consider the asymmetric character of LOCA transient. However, the level of details in the model must be balanced with computational capabilities.
- Refine the FP gap inventory calculations by considering differences between fuel rods/assemblies (i.e., provide multi-inventory, 3D burn-up distribution…) is also recommended.
- Regarding FP behaviour in containment, use of a dedicated calculation tool/module for modelling the complex and time dependent iodine behaviour/chemistry is necessary.

For SGTR transients

- Initial RCS contamination and spiking is of first importance. Real NPPs data can be preferred to be more realistic but it will be difficult to extend them to other operating or future NPPs (i.e. for different types of fuel, operating conditions…). Then, the development of more complex mechanistic models was recommended, at least in support of less detailed codes.
- All transport phenomena through SGTR break and in failed SG (atomization, flashing, partitioning, scrubbing) should be simulated based on feedback from the TH part. Iodine speciation in primary circuit conditions also (determining its volatility) as it could impact its flashing fraction at SGTR break and its partitioning from secondary liquid phase.
- For transfer to environment, as consequences of activity releases in liquid water or in steam phases are not the same, each phase must be considered separately in failed SG. In addition, for non-overflowing scenarios, aerosol retention in upper SG structure (size-dependent) must be calculated or deduced from the use of existing test facility results.

9 Uncertainty quantification

The evaluation of uncertainty is an integral part of the BE approach, and it is implicitly connected with the validation of the BE code. The adoption of a BE approach requests thus to evaluate the uncertainties connected with the elements of the analysis to derive the total uncertainty related to the code results in reproducing the behavior of the plant during the accident.

Uncertainty is generated by the unavoidable approximations in the data used to setup the code phenomenological models and in the implementation of these models in the code itself. Part of the uncertainty is also generated by the scaling issue related to the application of code models developed and validated using data obtained by scaled facility, to full scale NPP.

The progression of an accident occurring in a NPP is complex and complicated. Complex because a lot of phenomena take place, and the phenomena affect each other. Complicated because each single phenomenon typically depends on many quantities and is represented by complicated equations.
The use of software code implies the development of procedures and criteria regarding the use of the code itself, the setup of the model of the plant for the code and the data to be input. Particularly adopting the BE approach needs for evaluation of the uncertainties related to the obtained calculated results is generally requested.
Three major sources of uncertainty can be classified in these main groups:

- Phenomenological Models in the code.
- Representation and simulation of the plant for the code (limits and capabilities).
- Plant data uncertainty.

A list of code main uncertainty sources in codes was established during the project. More especially regarding LOCA and SGTR, the relevant phenomena/events occurring for both LOCA and DEC-A conditions (in RCS, containment, or SG) were listed and linked to the code sources of uncertainties. However, not all the phenomena and events have the same relevance for the target of the analysis. That is why, an evaluation (based on an expert opinion) of the relevance for uncertainty evaluation of the most relevant actions/phenomena (16 in total for both SGTR and LOCA) for uncertainty related to the considered scenario has also been established related to code capabilities and knowledge gaps. Challenging aspects were also included where:

- Code capability: is about the contribution to uncertainty due to capability in reproducing the action/phenomenon (e.g., adoption of empirical instead of mechanistic approach).
- Knowledge gap: is related to the knowledge of the phenomenological details of the action/phenomenon (e.g., lack in experimental tests and data).

The scaling issue

The setup and the validation of the phenomenological models in the codes are typically based on the experimental results performed in the test facilities. Data obtained in NPP are also used, but they cover only a small part of the range of the code phenomena models. Test facilities reproduce a part of the plant or specific phenomena (e.g., SETF) or the entire plant simulating the global behavior of the plant (ITF). In any case test facilities are scaled reproduction of the plant. The scaling process adopted in the design of the test facilities is characterized by a high level of complexity, because many aspects should be taken into account, but not all of them can be properly considered. Therefore, the model implemented in the code are for a certain extension affected by a scaling issue. The evaluation of the uncertainty contribution of the scaling issue is generally investigated comparing the uncertainty bands of the same accident/transient adopting different input scale. An important role in the scaling effect evaluation is played by non-dimensional parameters (NDP). Those parameters can be used for a comparison between the scaled facilities and the full-scale plant to identify the main aspects affected by the scaling. It makes possible to consider the distortions introduced in the facility compared with the NPP.

Overview of uncertainty evaluation approaches

In general terms the approaches adopted for the evaluation of uncertainty can be subdivided in two main groups. The relevant differences between the two approaches are related to the treatment of the calculation data to derive uncertainty. In “input uncertainty propagation” approach, the data of the calculations are generated by a proper statistical procedure to derive the uncertainty as the envelope of the possible results of selected calculations. In the “accuracy extrapolation” approach, the calculations results are used to derive the accuracy of the calculation, and with an extrapolation process the uncertainty is derived.

Figure **24** shows the scheme of the two strategies for the uncertainty evaluation.

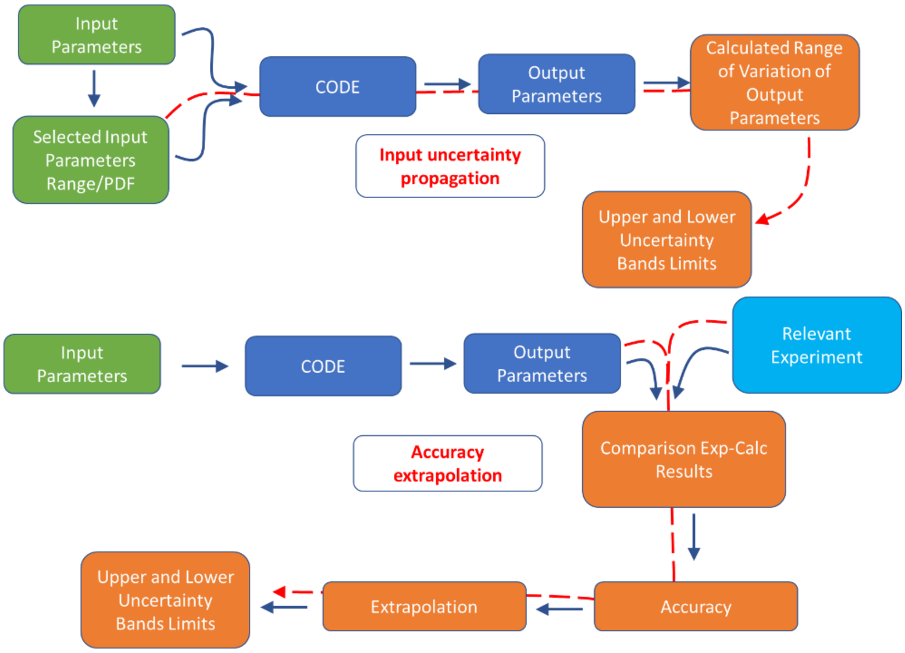


Figure 24: Simplified scheme of the uncertainty evaluation strategies

Input uncertainty propagation is focused on the propagation of uncertainties generated by input parameters. The input parameters are related to initial and boundary conditions, solutions adopted in the schematization of the plant, options of the phenomenological models of the code. The input uncertainties are propagated to the simulation model output uncertainties via the code calculations, with sampled data from known or assumed (classically probabilistic) distributions for key input parameters. This approach assumes that phenomenological models are properly qualified, and that the identification of the relevant input parameters is performed. Moreover, when it is based on the probability theory, it requires the choice of a PDF for each selected input parameters. In addition, special tools have been developed to apply this approach in an automatic way by coupling computer codes to probabilistic tools.
In the Accuracy extrapolation the effects of all uncertainty sources can be obtained by comparing experimental results performed in the test facilities with the code results in simulating those tests. The results of the comparisons between experimental and calculation results constitute the accuracy of the code in reproducing that test. Combining (extrapolation) the accuracy obtained in several calculations related to tests relevant for the analysis to be performed, the uncertainties to be applied at a best estimate analysis of the plant is evaluated.
Both approaches have advantages and weak aspects that should be taken into account (e.g., considering the level of knowledge of the considered phenomena, the availability of relevant experiments and data) that could suggest the preference of one approach instead of the other one.

Proposal for global uncertainty approach

As seen in the previous sessions, the evaluation of the RC is a complex process requiring several phenomena to be modelled and involving different technological areas and related tools. The uncertainty related to the interface adopted to transfer data between the coupled codes has to be then also considered.
Figure **25** is reported the scheme of the coupled calculations and the transferring of data between them.

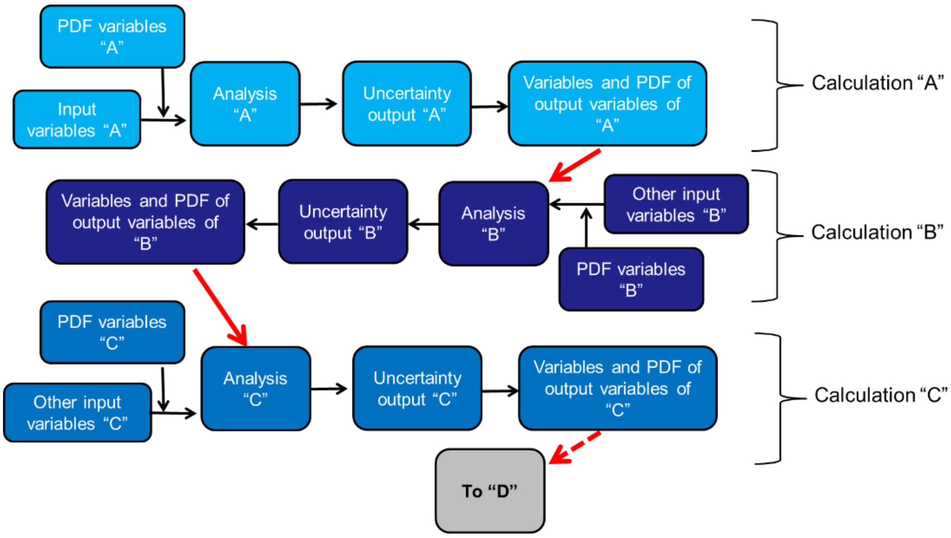


Figure 25: Broad scheme for execution of coupled calculations

In addition to the uncertainty of the calculation output the uncertainty due to the interface between codes should also be included:

- Uncertainty due to spatial discrepancy
- Uncertainty related to time discrepancy
- Uncertainty related to data format discrepancy

Performing sensitivity analyses and uncertainty quantification for all the updated calculations provided was beyond the scope of the project. However few sensitivity analyses and uncertainty quantification (using different methodologies) have been performed within the project for dedicated phenomena. An Uncertainty Quantification of the I-131 transport up to the environment during a SG scenario was in particular carried out by extending the use of the CIAU code (based on Accuracy Extrapolation Methodology) [42]. This method is, currently used to determine the uncertainty of thermalhydraulic transient simulations and only requires, contrarily to other uncertainty evaluation methods, one (best-estimate) transient simulation, the results of which is afterwards compared with the weighted average of a set of experimental data of NPPs. Therefore, only combinations of parameters that actually occurred are considered.
Regarding uncertainty on iodine transport, as not enough data are available it was derived from the basic thermohydraulic parameters of the CIAU method. The propagation of uncertainty method indeed allowed to extend the uncertainty calculations done by the CIAU analysis from the primary system to the secondary system and then to the environment without having experimental data on iodine transport. The transport of iodine into the environment was shown to be the subject to a very pronounced uncertainty (**Figure 26**).

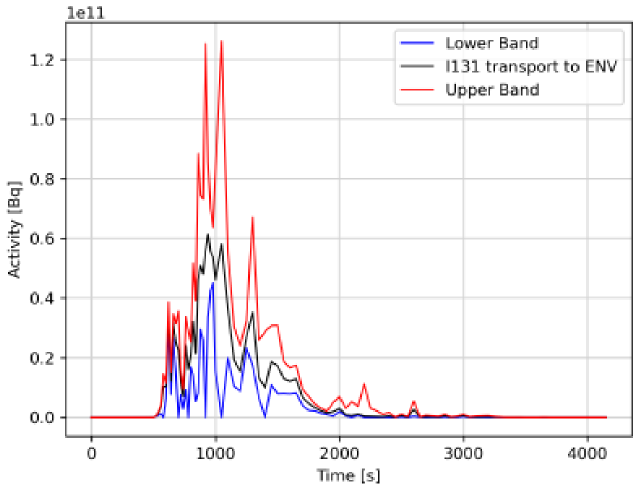


Figure 26: CIAU evaluation of the uncertainty on I131 releases in the environment in SGTR DEC-A scenario in VVER-1000

10 Main Progresses in Accident Management and Prevention

Several studies were performed to cope with the radiological consequences of SGTR, resulting in containment by-pass with direct release of radioactive coolant to the environment. It concerned the development of new automatic safeguards algorithms or their optimization as well as the detection of defective fuel rods in a core.

10.1 AMP optimisation

Automatic safeguards algorithms to cope with primary to secondary breaks similar to the one implemented in GenIII+ VVER NPP design at older VVER-1000/V320 NPPs were developed within the project and evaluated based on quantitative analysis of SGTR transients. Indeed, though several designs of the algorithms were already available they, to a large extent, involved normal operation systems. The objectives of these developed algorithms were to automatize the needed prompt actions not degrading the main unit safety functions till NPP stabilisation using primarily the safety systems with no or minimal use of normal operations systems and need for operator interventions. Application of these algorithms made it possible to eliminate or minimize the FP release to environment whatever the SGTR DBA transients was considered, to ensure the stabilisation of the emergency process and to create e a sufficient reserve of time for operational personnel to perform further emergency management actions, if needed.

In parallel, a general approach of optimizing an Accident Management Procedure (AMP) [47], earlier applied to a station blackout in VVER1000 [50], was refined in the frame of the R2CA project and applied to a SGTR scenario for a generic PWR, four loops, 3750 MWth. The accident management strategy for such events currently aims at reducing the primary system pressure as fast as possible to prevent further loss of coolant to the secondary system. To achieve this goal, several actions can be done by the operator. The Downhill Simplex Method [51] was used to optimize the timing of the operator actions: such as opening of the PORV, disconnection of train 3 and 4 of HPIS. The Method provides a very robust numerical algorithm to find a local minimum of a function $F:\mathbb{R}^n \rightarrow \mathbb{R}$. First step is to create an initial, arbitrary simplex in $\mathbb{R}^n$ (i.e. the simplest geometrical shape, e.g. a triangle in $\mathbb{R}^2$ or a tetraeder in $\mathbb{R}^3$). The function F is then evaluated at each corner of the simplex. The highest point is moved according to the algorithm and a new simplex is constructed, the function is again evaluated, and so on. The series of simplexes slowly converges to a local minimum. To use the simplex method for AM optimization, the independent parameters of the function were chosen to be the timing of the three above mentioned operator actions. Then, a thermal hydraulic system code (the function) evaluated the plant response. As dependent variable, a figure of merit was constructed, that evaluated the AM-Measures based on a.) the radioactive releases to the environment, b.) the primary pressure at the end of the transient and c.) the water level in the reactor core. A higher score meant a worse performance; a lower score translated to low releases, low primary system pressure, and good coverage of the reactor core throughout the transient. The simplex method was then applied to find the optimum timing for the operator actions. After thirteen iterations, the algorithm converged to a minimum. The results showed that the opening of the PORV is most efficient later in the transient, while shutting down one HPIS early, and the second one late in the transient, provides good results. Overall, the release of iodine to the environment could be reduced by several orders of magnitude, applying the right timing of the investigated operator actions (**Figure 27**).

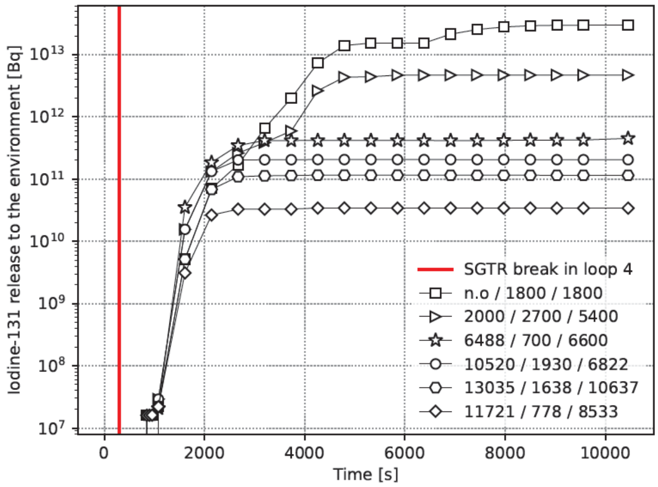


Figure 27. Iodine release in environment as a function of operator action timing

10.2 Neural Networks for early accident diagnosis

In case of fuel defects, activity is released in the primary coolant of PWR. Some data-driven methods, especially machine learning and deep learning approaches for fuel defect detection have gained momentum in the recent years. Artificial neural networks (ANN) have started to be used in the two last decades and gave good results, but since they are not meant to intake time related data, there can be sometimes false negatives. On the contrary, recurrent neural networks or related methods like Gated Recurrent Units networks (GRU) [54] or Long Short Term Memory (LSTM) networks [55] are designed to deal with time dependent data. R2CA project gave the opportunity to test these methods on synthetic data.

On a first step, a simple physical model was built to generate physical data: The physical model was developed using the mass balance equations in the three regions (pellet, gap, and coolant), to get the estimates of radioisotope activities in the primary coolant.

In the fuel pellet the release is dominated by mechanisms such as recoil, knockout and diffusion. Unlike diffusion, recoil and knockout release are athermal processes (dominant below about 1000°C). Knockout is of little importance compared to that of recoil and for this reason, has been neglected. The expression for the recoil release is adapted from [56]. For the diffusion release within the fuel pellet, we used the from model from [52, 58]. The diffusion coefficient, involving high, intermediate and low-temperature effects was the one proposed by [59].

When the fuel cladding is defective, the coolant can enter the gap and flash into water steam. Due to the pressure pulsation caused by the flashing and occurrence of steam-oxidation of the UO_2 fuel, the release of the fission products can be enhanced [57]. This transient release is not considered in the present study and only the long-term steady state release is modeled, using [60] model.

At last, the fission products transport in the coolant was modelled using the first-order kinetic approach. The source terms are the release from the gap to the coolant and the release from tramp uranium, whereas the loss term comprises the decay of radioisotopes and the contribution from different purification systems located in the primary coolant circuit (**Figure 28**).

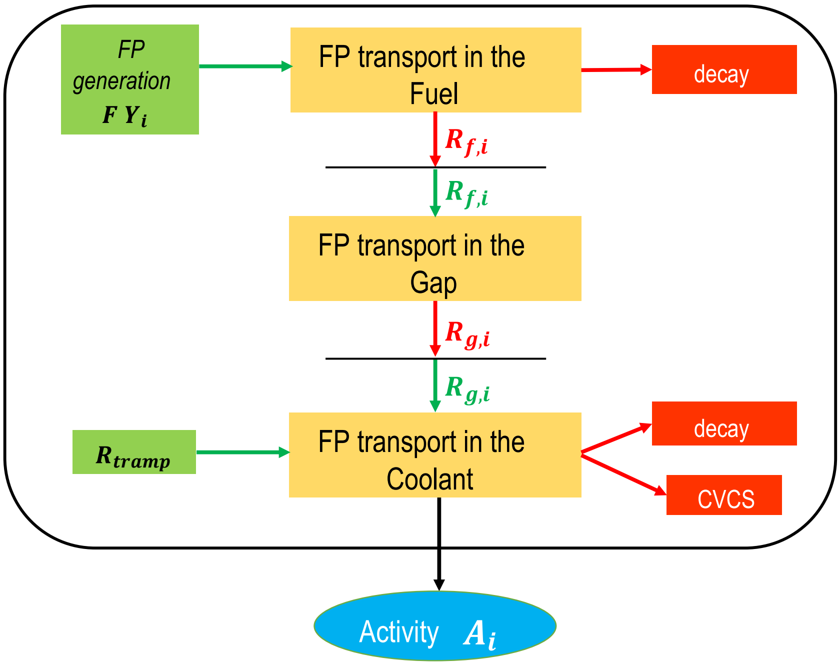


Figure 28: Schematic diagram for production and loss through the Fuel, Gap and Coolant and eventual coolant activity estimation.

This model showed satisfactory behavior in the computation of 8 decay chains comprising a total of 30 radioisotopes. These decay chains were considered as they comprised the isotopes of interest such as noble gases (Xe, Kr) and volatile species (I). In the pellet region, the results were in accordance with the results observed by sweep gas experiments [53, 56]. In the gap region, the different escape regimes From (Veshchunov, 2019) were noted for the different isotopes in the gap region.

Having a physical model to calculate the radioisotope activities in the coolant, the production of the database could be done by varying the input parameters of the model (power, temperature, inlet and outlet flow rates of the primary circuit, etc.), to get the different output (activity) values at different times before and after defect onset. For that part of the work, the computations involved only the I131 decay chain, due to CPU considerations. Additionally, even if the model is simple and fast, the amount of data needed to feed the training recurrent networks has proven to be excessive regarding the precision to be achieved. Instead, it was decided to build a surrogate model of the I131 decay chain, which ended with a good precision model. 2000 physical calculations were done and fed to machine learning devices (ANN in case of defect, Lasso method using polynomial features in absence of defect). Among these 2000 sequences, 1500 were used for training, and 500 were left apart for the test phase. On the test data, the models performed with a precision higher than 99%.

The surrogate model was then used to generate 50000 activity sequences. The time step of the sequences was considered an import matter, as it represents the sampling rate measurement in real life applications. So different time steps were tested, spanning from 1 hour to 24 hours, which resulted 5 sets of 50000 sequences. Another important matter was also taken into consideration, the length of the sequences (number of time steps in the sequence). As one would like to reduce the amount of data of a sequence as much as possible, various sequence lengths were tested, 3,4-time steps, multiplying by a factor 2 the number of 50 000 sets.

This led to 30 models of defect detection (GRU, RNN, LSTM); for each of them, 5 times steps; and for each of these, sequence length of ¾ time steps.

100% accuracy was achieved by all methods applied to all time step/sequence length configuration (**Figure 29**).

We found however that LSTM and GRU learn faster than recurrent networks.

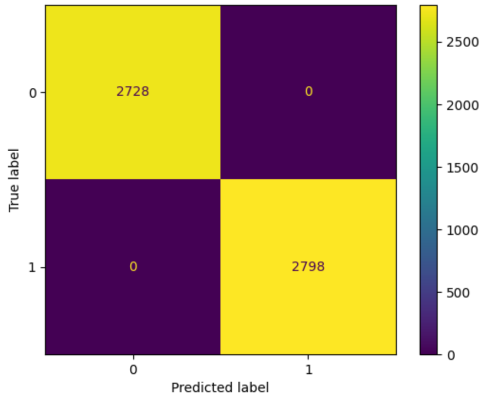


Figure 29: Confusion matrix example for LSTM, with 1 hour time step and 3-time steps per sequence

The interesting outcomes are the following:

- A physical model than can generate activity data due to defects was built; as it is simple but yet renders credibly the behavior of the real physical system, it could be used by anyone to benchmark the efficiency of fault detectors (the whole content of this model is to be published in a special issue of Annals of Nuclear Energy.
- The method for the construction of a reasonable CPU intensive calculation chain has been built; it involves surrogate models, quite precise when staying in the parameter space of the initial physical model.
- AI methods used in other industrial fields have been tested and validated.

11 Exploratory work on ATF evaluation

Following the accident in Fukushima-Daiichi, many large international research and development activities have been launched to develop enhanced Accident Tolerant Fuel (ATF) cladding materials for Light Water Reactors (LWRs). The global objectives of ATFs are to enhance the safety margins, for both severe accident as well as design basis accidents, while maintaining the commercial performance of current LWR fuels. During a design basis loss of coolant accident (LOCA) scenario, an increase of the inner cladding pressure and a loss of outer cladding pressure occurs. Combined with the presence of high temperature steam, the cladding undergoes ballooning and burst.

The international community provided several overviews of the outcomes of the research [61-66]. The JRC took part in the review of alumina forming alloys, such as FeCrAl, ODS steels, SiC-SiC composite materials and MAX phase material analysed in the frame of the Il Trovatore project [67-69]. The analysis covered the static autoclave tests under PWR conditions, showing excellent performance of currently used zirconium alloys and that chromia showed the lowest corrosion rate after zirconia. Furthermore, steam oxidation tests at KIT performed at 1200°C also revealed the low reaction rates of SiC and that FeCrAl showed a high resistance against steam oxidation [69].

One of the main near-term candidate materials that stand out are the Cr-coated zirconium-based cladding materials. In the frame of the R2CA project, a bibliographic survey was prepared [70]. The review started with the various chromium coating processes currently applied such as physical or chemical vapour deposition, cold spray and 3D laser-melt coating. Must of theses coatings techniques are currently used by fuel vendors Framatome

(PVD), Westinghouse Electric Corporation in the US (PVD and CS), and in South Korea (Laser Melt Coating). In addition, some of the advances in coating technologies were summarised.
The review of material properties then covered thermal properties (thermal expansion, diffusivity, conductivity, and heat capacity at constant pressure), mechanical properties for both normal operating conditions as well as at high temperature for loss of coolant conditions, corrosion resistance and the effects caused by radiation.

Based on the review, a first assessment was made during the project of the Cr-coated cladding materials under LOCA conditions by means of the DRACCAR code, comparing standard fuel with Zry and the coated cladding material under LOCA conditions. More precisely, they re-assessed the QUENCH L1 case from the QUENCH LOCA program of KIT, which was applied in the coordinated research project (CRP) of the IAEA FUel Modelling under Accident Conditions (FUMAC). For this purpose, the creep rate of Zry-4 was divided by a factor 2, the same burst stress criterion of standard Zry-4 was applied, and the same oxidation model was also considered. A maximum strain in the ATF-like material that is about half that of standard Zry-4 along was obtained with a delayed burst that was consistent with experimental observations, despite the large scatter in the experimental data in terms of circumferential strain and position of the burst. A similar assessment was made with DRACCAR based on the IFA-650.10 case of Halden, which was also applied in the FUMAC benchmark of the IAEA. Adopting the same assumptions, a slight delay of the burst in Cr-coater Zry in comparison with the standard cladding was also shown.

The impact of Cr-coated Zry cladding materials during LOCA conditions was also assessed by means of a sensitivity study with the FRAPTRAN code on the basis of a large break LOCA scenario with a maximum peak cladding temperature of 1189ºC and equivalent cladding reactor of 6.76%. The simulations considered a reduced corrosion and high temperature oxidation, a finite element analysis model with NUREG 0630 burst strain model or user defined rupture strain, and a reduced annealing rate. Nevertheless, some code modifications are still required to be able to reproduce the reduced burst strain of Cr-coated claddings, including a high temperature creep law.

Finally, some material properties for various ATF materials were upgraded in TRANSURANUS. In collaboration with different partners [71], [72], [73-74] the properties for U_3Si_2 fuel and FeCrAl cladding material properties have been implemented progressively and assessed on the basis of a case from the CRP FUMEX-II. In addition to estimating the impact of new material properties on the fuel performance, an uncertainty analysis for the ATF material properties was also performed by means of the built-in Monte Carlo approach in TRANSURANUS. Analysis of the outcome by means of the TUPython tool allowed to evaluate the impact of the uncertainties of the ATF properties, and to evaluate the relative impact by means of the Pearson coefficient. A similar task was carried out in collaboration with the University of Cambridge for the material properties for Hastelloy-n cladding [75]. In a next phase, also Cr-coated Zircaloy will be simulated by means of the TUmech [76] tool that has been created in the frame of a collaboration with CIEMAT. Nevertheless, the publication of this work with Cr-coated cladding will be out of the timeframe of the R2CA project.

12 Knowledge dissemination and E&T

R2CA communication activities towards the general public and stakeholders were to promote the project work, to link it to the societal values and to demonstrate added value for the EU. The communication and dissemination of R2CA project and results have been oriented towards the widest community as possible, so the results have been made accessible to the general public. The transfer of the consolidated knowledge and of project results to young researchers has been one of the key tasks of the project, as well.

The target group identified has been general public, nuclear scientific community and more especially thermal-hydraulic, fuel and source term community, international Organization and networks (IAEA, OECD-NEA, ETSON, SNETP, ...), TSO community, emergency preparedness and response community, regulator community, NPP owner community, vendors, master and PhD students. Considering the different audiences of the projects, the communication and dissemination strategy included different means and channels to try to arouse the widest interest. Several different tools or actions have been considered detailed below. Some of these actions could unfortunately not be carried out during the COVID health crisis.

R2CA PUBLIC WEB SITE & ZENODO REPOSITORY

The R2CA project website (Public area) has been created at the beginning of the project and has been continuously updated throughout the project duration. The link for the website is the following https://r2ca-h2020.eu/index.html and it contains: a short description of the project (https://r2ca-h2020.eu/about.html), project partners (https://r2ca-h2020.eu/projects_partners.html), newsand event (https://r2ca-h2020.eu/news_events.html) a short description of the different WP, (https://r2ca-h2020.eu/activities.html), public documents and publications (https://r2ca-h2020.eu/documents_publications.html). In parallel, an open-access repository where the R2CA public deliverables and publications was archived, was also created on Zenodo (Search results (zenodo.org)).

ORGANISATION OF INTERNATIONAL OPEN WORKSHOPS

Considering the COVID issue, only one final international workshop has been organized to disseminate among the international scientific community the main achievements of the project. It has been opened to researchers from non-partner-organizations. H**eld the 29-30 November in IRSN headquarters Fontenay-aux-Roses, France,** it discussed the main results and outcomes of the project dedicated to Design Basis and Design Extension of Loss-Of-Coolant and Steam Generator Tube Rupture Accidents, Accident Management and Procedures, Innovative Tools and Devices. Main topics addressed were: fuel/clad thermomechanics, FP releases from fuel, FP transport and physico-chemical behaviour, calculation methodologies & radiological consequence assessments of LOCA and SGTR transients. Accident Tolerant Fuel evaluation, optimisation of Accident Management & Prevention procedures and the potential of Artificial Intelligence based methods for anticipating accidental configurations were also discussed.

Figure 30: Agenda of the R2CA Open Workshop

ELECTRONIC NEWSLETTERS

Four yearly electronic newsletters have been released to inform the stakeholders of the project advancements and the main activity/results. These have been shared through LinkedIn (ResearchGate was also used till March 2023). Newsletters have been shared through the partners and will be uploaded on the R2CA website.

PUBLIC DELIVERABLES

Amongst the deliverables provided by the project 16 technical reports were public and were (or will be) archived in both the R2CA public website and the Zenodo repository (**Table 1**).

Task	Deliverable	Technical Content
1.1	D1.8	Final project synthesis activity report
2.1	D2.1	LOCA and SGTR DBA and DEC-A available evaluation methodologies
2.1	D2.2	LOCA and SGTR available simulation codes
2.1	D2.3	LOCA and SGTR available experimental data
2.4	D2.6	Uncertainty analyses
2.5	D2.7	Reassessment of reactor tests cases
2.6	D2.8	Updated harmonized methodologies
3.1	D3.2	Final report on fission product relase during LOCA
3.2	D3.4	Final report on rod cladding failure during LOCA
3.3	D3.6	Final report on fuel rod behaviour during LOCA
4.1	D4.2	Final report on fission product release during SGTR
4.2	D4.4	Final report on rod cladding failure during SGTR
4.3	D4.5	Failure criteria for defective fuel rods during SGTR
5.1	D5.1	Report on Pro and Cons of innovative devices and management approaches
5.2	D5.2	Report on innovative diagnosis tools and devices
5.3	D5.3	Report on Pro and Cons of ATF

Table 1: Public deliverables published along the R2CA project

TRAINING AND SUMMER SCHOOLS

An important objective of the R2CA project was to contribute to the European effort on nuclear education and training activities. In this respect, 4 training courses have been organized on dedicated codes used within the project (SCIANTIX, DRACCAR, TRANSURANUS, TRANSURANUS + SCIANTIX) as well as a Summer School.

Code / subject	Duration	Period	Host organization
TRANSURANUS Fuel Performance Code	1 week	January 17-21, 2022 (Karlsruhe)	JRC-Ka
SCIANTIX Meso-scale code for FG behavior in fuel	1 day	October 16, 2020 (on-line)	ENEA-POLIMI
DRACCAR 3D fuel/clad thermomechanical code	2 days	September 9-20, 2022 (Bologna)	ENEA-IRSN
TRANSURANUS*SCIANTIX/MFPR-F Fuel Performance and FG coupled code	1 week	June 26-30, 2023 (Karlsruhe)	JRC-Ka

Table 2: Training courses organised along the R2CA project

SCIANTIX TRAINING

On October 16, 2020, the first online SCIANTIX Training Course was held. SCIANTIX is an opensource code devoted to the simulation of inert gas behaviour within nuclear fuel, designed for inclusion in fuel performance codes. In the frame of R2CA, SCIANTIX was extended to also model the production and transport of fission products within the fuel pellet. The training included a general introduction to physics-based modelling of inert gas behaviour and proposed hands-on case studies for the participants to directly use SCIANTIX. The 30+ participants to the training came from both institutions within and outside the consortium of R2CA. The material used in the Training (slides, case studies with related documentation) has been publicly available, together with the source code of the SCIANTIX version used.

TRANSURANUS

On January 17-21, 2022, the TRANSURANUS training course was held in Karlsruhe. The training course was organised and hosted by the JRC for 12 young academic staff from Technical Safety Organisations, research centres, universities and industry that included 3 organisations from R2CA. It gave a theoretical basis on nuclear fuel behaviour in a nuclear reactor. It showed how to prepare and use the TRANSURANUS code for various fuel performance analyses. During the course, the TRANSURANUS code was used for analysing thermal and mechanical behaviour of the nuclear fuel in the reactor and for analysing behaviour of gaseous fission products. Furthermore, the trainees learned to implement new model parameters in the source code and create a new executable version and also to verify compliance with safety and design criteria provided by the IAEA.

DRACCAR TRAINING

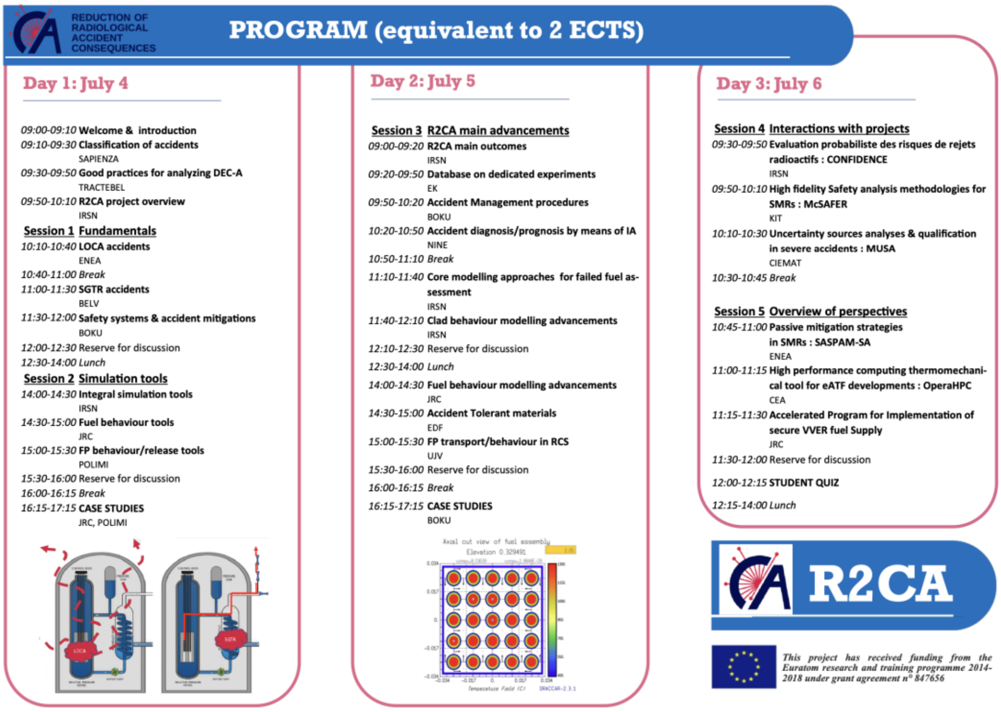
On September 19-20, 2022, a “beginner” course on DRACCAR code was held in Bologna. The training course was organized by IRSN and hosted by ENEA. The DRACCAR computer code, developed by IRSN since 2006, is used for the safety analysis of PWRs and in support to research programs on fuel rod behavior during a LOCA. DRACCAR is a multi-rod 3D simulation tool coupling the thermohydraulic of fuel assembly sub-channels and the thermomechanical behavior of fuel rods during LOCA. 15 participants from organizations participating to the project attended the training course.

TRANSURANUS * SCIANTIX / MFPR-F

On June 26-30, 2023, another training on TRANSURANUS was organized, but this time dedicated to its coupling with the new SCIANTIX 2.0 version from POLIMI and the MFPR-F code from IRSN, both further improved within the R2CA project. The training course took place in Karlsruhe for 8 participants. The training provided an introduction on the three codes, focusing on the SCIANTIX capabilities and its functioning as a fission gas behaviour module within the TRANSURANUS fuel performance code, complemented with an online introduction about the fission product chemistry capabilities of the MFPR-F code. The participants had the opportunity to employ the coupled code suite TRANSURANUS-SCIANTIX to analyse representative LWR fuel rods and investigate the code calculations in terms of integral fission gas release provided by SCIANTIX.

R2CA Summer school

On July 4-6, 2023, a Short Summer School has been organized by ENEA and IRSN in Bologna. The main target of the summer school was to disseminate the knowledge consolidated and gained along the R2CA project to Master and PhD students, young researchers and engineers involved in nuclear energy and reactor safety analyses. Along the school the main safety aspects related to DBA and DEC-A of LOCA and SGTR accidents have been discussed focusing the attention on the phenomenology, experimental knowledge available and current numerical modelling. Main advancements within the R2CA project served as a background to show the current state of art and the new ideas. The school targeted both fundamental knowledge, current nuclear safety best practices and innovation. A video has been done to summarize the event.



REDUCTION OF RADIOLOGICAL ACCIDENT CONSEQUENCES

PROGRAM (equivalent to 2 ECTS)

Day 1: July 4

09:00-09:10 **Welcome & introduction**
09:10-09:30 **Classification of accidents**
SAPIENZA
09:30-09:50 **Good practices for analyzing DEC-A**
TRACTEBEL
09:50-10:10 **R2CA project overview**
IRSN
Session 1 Fundamentals
10:10-10:40 **LOCA accidents**
ENEA
10:40-11:00 Break
11:00-11:30 **SGTR accidents**
BELV
11:30-12:00 **Safety systems & accident mitigations**
BOKU
12:00-12:30 Reserve for discussion
12:30-14:00 Lunch
Session 2 Simulation tools
14:00-14:30 **Integral simulation tools**
IRSN
14:30-15:00 **Fuel behaviour tools**
JRC
15:00-15:30 **FP behaviour/release tools**
POLIMI
15:30-16:00 Reserve for discussion
16:00-16:15 Break
16:15-17:15 **CASE STUDIES**
JRC, POLIMI

Day 2: July 5

Session 3 R2CA main advancements
09:00-09:20 **R2CA main outcomes**
IRSN
09:20-09:50 **Database on dedicated experiments**
EK
09:50-10:20 **Accident Management procedures**
BOKU
10:20-10:50 **Accident diagnosis/prognosis by means of IA**
NINE
10:50-11:10 Break
11:10-11:40 **Core modelling approaches for failed fuel assessment**
IRSN
11:40-12:10 **Clad behaviour modelling advancements**
IRSN
12:10-12:30 Reserve for discussion
12:30-14:00 Lunch
14:00-14:30 **Fuel behaviour modelling advancements**
JRC
14:30-15:00 **Accident Tolerant materials**
EDF
15:00-15:30 **FP transport/behaviour in RCS**
UJV
15:30-16:00 Reserve for discussion
16:00-16:15 Break
16:15-17:15 **CASE STUDIES**
BOKU

Axial cut view of fuel assembly
Elevation 0.329491

Day 3: July 6

Session 4 Interactions with projects
09:30-09:50 **Evaluation probabiliste des risques de rejets radioactifs : CONFIDENCE**
IRSN
09:50-10:10 **High fidelity Safety analysis methodologies for SMRs : McSAFER**
KIT
10:10-10:30 **Uncertainty sources analyses & qualification in severe accidents : MUSA**
CIEMAT
10:30-10:45 Break

Session 5 Overview of perspectives
10:45-11:00 **Passive mitigation strategies in SMRs : SASPAM-SA**
ENEA
11:00-11:15 **High performance computing thermomechanical tool for eATF developments : OperaHPC**
CEA
11:15-11:30 **Accelerated Program for Implementation of secure VVER fuel Supply**
JRC
11:30-12:00 Reserve for discussion
12:00-12:15 **STUDENT QUIZ**
12:15-14:00 Lunch

R2CA

This project has received funding from the Euratom research and training programme 2014-2018 under grant agreement n° 847656

Figure 31: R2CA summer school agenda

PUBLICATIONS IN PEER REVIEW JOURNAL AND CONFERENCE PROCEEDINGS

In order to share with the nuclear stakeholders the progress made in the R2CA project and to reach the largest possible audience, the results of the projects have been presented in international scientific conferences, workshop, and published in peer reviewed publications.

A dedicated special issue on the Annals of Nuclear Energy Journal has also been organized in order to collect all the outcomes of R2CA project. It helped enhancing the visibility of the activities and maximizing the impact of the project. The special issue is under finalization. The guest editors are Nathalie Girault, Fulvio Mascari, Lelio Luzzi (https://www.sciencedirect.com/journal/annals-of-nuclear-energy/special-issue/105M36PSDR6)

Below is a small summary of some of the papers published along the project.

- R. Calabrese, A. Schubert, et alt., “M5 cladding material: reviews of models relevant for LOCA simulation”, **International Conference Nuclear Energy for New Europe NENE2021**, Bled (Slovenia) September 6 - 9, 2021.
- Zamakhaeva, A. Kecek, “Adsorption of iodine on painted surfaces in Nuclear Power Plants containment buildings”, **International Conference Nuclear Energy for New Europe NENE2021**, Bled (Slovenia) September 6 - 9, 2021.
- F. Feria, C. Aguado, et alt., “Effect of hydrogen precipitation on in-clad hydrides distribution in irradiated fuel rods”, **Annual Meet. of the Spanish Nuclear Society 2021**, Granada (Spain), 2021
- R. Iglesias, L. E. Herranz, et alt., “Modeling SGTR DEC-A sequences with the MELCOR Code**”, Annual Meeting of the Spanish Nuclear Society 2021**, Granada (Spain), 2021.
- Z. Soti, P.V. Uffelen, et alt., “Extending the application of TRANSURANUS to coupled code calculations and statistical analysis”, **TOPFUEL 2021**, Santander (Spain) 24-28 October 2021.
- Z. Hózer, P. Szabó, et al., “Review of experimental databases for SGTR and LOCA analyses”, **TOPFUEL 2021**, Santander (Spain) 24 - 28 October 2021.
- F. Feria, L.E. Herranz, “Scoping calculations of in-clad hydrides distribution under secondary hydriding in defective fuel rods”, **TOPFUEL 2021**, Santander (Spain) 24 - 28 October 2021.
- G. Zullo, D. Pizzocri, et alt., “Coupling of SCIANTIX and TRANSURANUS: Release of radioactive fission products”, **International Workshop for TRANSURANUS** Users and Developers 2021.
- F. Kremer, R. Dubourg, “Applications of the coupling between TRANSURANUS and MFPR-F”, **International Workshop for TRANSURANUS** Users and Developers 2021.
- R. Zimmerl, L. Anzengruber, et alt., “Code to experiment comparison of a steam generator hot header break at PSB-VVER test facility with RELAP5/SCDAP 4.1 thermal hydraulic system code”, **International Topic meeting on Nuclear Reactor Thermal Hydraulics, NURETH19**, Brussels (Belgium), 6-11 March, 2022.
- T. Kaliatka T. Kacegavicius, P. and A. Kaliatka, “Analysis of LOCA Accident for BWR-4 under DEC-A conditions using ASTEC code”, the **10th European Review Meeting on Severe Accident Research (ERMSAR 2022)**, Akademiehotel, Karlsruhe, Germany, May 16-19, 2022.
- N. Girault et alt., “The R2CA project for evaluation of radiological consequences at design basis accidents and design extension conditions for LWRs: Motivation and first results”, the **10th European Review Meeting on Severe Accident Research (ERMSAR 2022)**, Akademiehotel, Karlsruhe, Germany, May 16-19, 2022.
- R. Iglesias, L. E. Herranz, “Extension of the MELCOR code to DEC-A SGTR scenarios”, **47th Annual Meeting of the Spanish Nuclear Society,** 28-30 September, Cartagena, Spain.
- R. Calabrese, “Crystallographic phase transition of zirconium alloys: simulation of LOCA accidents with the TRANSURANUS code”, **31st International conference Nuclear Energy for New Europe, NENE2022**, Portoroz 12-15 September 2022.
- P. Van Uffelen, A. Schubert, Z. Soti, “Assessing the effect of some ATF material and uncertainties on their properties under normal conditions by means of the TRANSURANUS code”, **PBNC 2022**, Chengdu, China, October 30 – November 4, 2022.
- G. Zullo, D. Pizzocri, et alt., “On the use of spectral algorithms for the prediction of volatile fission product release: Methodology for bounding numerical error”, **Nuclear Engineering and Technology**, 54 (2022) 1195-1205.
- G. Zullo, D. Pizzocri, et alt., “Towards grain-scale modelling of the release of radioactive fission gas from oxide fuel. Part I: SCIANTIX”, **Nuclear Engineering and Technology**, 54 (2022) 2271-2782.
- G. Zullo, D. Pizzocri, et alt., “Towards grain-scale modelling of the release of radioactive fission gas from oxide fuel. Part II: Coupling SCIANTIX with TRASURANUS”, **Nuclear Engineering and Technology**, 54 (2022) 4460-4473.

- F. Kremer, A. Tidikas, A. Slavickas, "Progress in the modelling of high burn-up structure: application of the TRANSURANUS/MFPR-F coupling to NRC-192 STUDSVIK LOCA test", **TOPFUEL 2023**, Xi-an (China) 18-21 July 2023.
- B. Dif, A. Arkoma, J. Heikinheimo, 'Re-evaluation of FRAPTRAN cladding failure criterion in LOCA within R2CA project", **WRFPM 2023**, Xi-an (China) 18-21 July 2023.
- M. Jobst, E. Diaz-Pescador, S. Kliem, "Core Damage Extent Analysis of Large-Break LOCA for 4-Loop Pressurized Water Reactor with Detailed 3D Model of Reactor Pressure Vessel and Core**", International Topic meeting on Nuclear Reactor Thermal Hydraulics, NURETH20**, Washington (USA), 20-25 August, 2023.
- L. Verma, F. Kremer, K. Chevalier-Jabet, "Defective PWR fuel rod detection and characterization using an Artificial Neural Network", Progress in Nuclear Energy, 160 (2023) 104686.
- G. Zullo, D. Pizzocri, L. Luzzi, « The SCIANTIX code for fission gas behaviour: status, upgrades, separate-effect validation and future developments", **Journal of Nuclear Materials**, 587 (2023) 154744.

ANE special issue papers: up to now these are the papers published, others are under review:

- F. Feria, L.E. Herranz, "Assessment of hydride precipitation modelling across fuel cladding: Hydriding in non-defective and defective fuel rods", Annals of Nuclear Energy, Volume 188, 2023, 109810.
- G. Zullo, D. Pizzocri, L. Luzzi, F. Kremer, R. Dubourg, A. Schubert, P. Van Uffelen, "Towards simulations of fuel rod behaviour during severe accidents by coupling TRANSURANUS with SCIANTIX and MFPRF", Annals of Nuclear Energy Volume 190, 2023, 109891.
- A. de Lara, A. Schubert, E. Shwageraus, P. Van Uffelen, "Towards preliminary design calculations with TRANSURANUS for application of Hastelloy cladding material", Annals of Nuclear Energy, Volume 192, 2023, 109973.
- Z. Hózer, M. Adorni, A. Arkoma, V. Busser, B. Bürger, K. Dieschbourg, R. Farkas, N. Girault, L.E. Herranz, R. Iglesias, M. Jobst, A. Kecek, C. Leclere, R. Lishchuk, M. Massone, N. Müllner, S. Sholomitsky, E. Slonszki, P. Szabó, T. Taurines, R. Zimmerl, "Review of experimental database to support nuclear power plant safety analyses in SGTR and LOCA domains", Annals of Nuclear Energy, Volume 193, 2023, 110001.
- A. Berezhnyi, A. Krushynskyi, D. Ruban, S. Sholomitsky, "Conservative evaluation of radionuclides release for VVER-440 and VVER-1000 type reactors", Annals of Nuclear Energy, Volume 194, 2023, 110105.
- Tadas Kaliatka, Tomas Kačegavičius, Algirdas Kaliatka, Mantas Povilaitis, Andrius Tidikas, Andrius Slavickas, "Methods for the radioactive release estimation under DEC-A conditions", Annals of Nuclear Energy, Volume 195, 2024,110143.
- F. Feria, P. Aragón, L.E. Herranz, Assessment of cladding ballooning during DBA-LOCAs with FRAPTRAN, Annals of Nuclear Energy, Volume 195, 2024,110194
- A. Bousbia Salah, M. Di Giuli, P. Foucaud, R. Iglesias, A. Malkhasyan, M. Salmaoui, L.E. Herranz, "Iodine source term assessment under DBA SGTR accident scenario", Annals of Nuclear Energy, Volume 196, 2024,110201.
- L. Giaccardi, M. Cherubini, G. Zullo, D. Pizzocri, A. Magni, L. Luzzi, "Towards modelling defective fuel rods in TRANSURANUS: Benchmark and assessment of gaseous and volatile radioactive fission product release", Annals of Nuclear Energy, Volume 197, 2024,110249.
- P. Foucaud, M. Di Giuli, M. Salmaoui, A. Bousbia Salah, R. Iglesias, A. Malkhasyan, L.E. Herranz, "Iodine source term assessment as result of iodine spiking and mass transfer phenomena during a SGTR transient using MELCOR 2.2 and CATHARE 2 codes", Annals of Nuclear Energy, Volume 198, 2024, 110305.

COMMUNICATION MATERIAL

Logo and Document Template: They were built at the beginning of the project to identify and give visibility to the project.

Design of Material to Support Project Dissemination and Communication Activities: A R2CA project brochure and poster have been designed at the beginning of the project. The brochure was distributed, and the poster displayed at various events to promote the project and increase its visibility towards stakeholders or civil society (**Figure 32**, **Figure 33**).

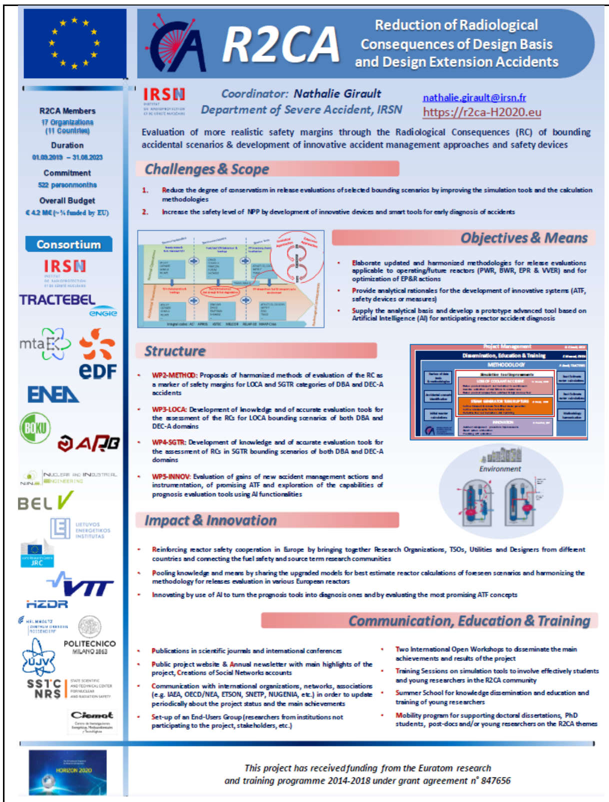


Figure 32: R2CA Poster

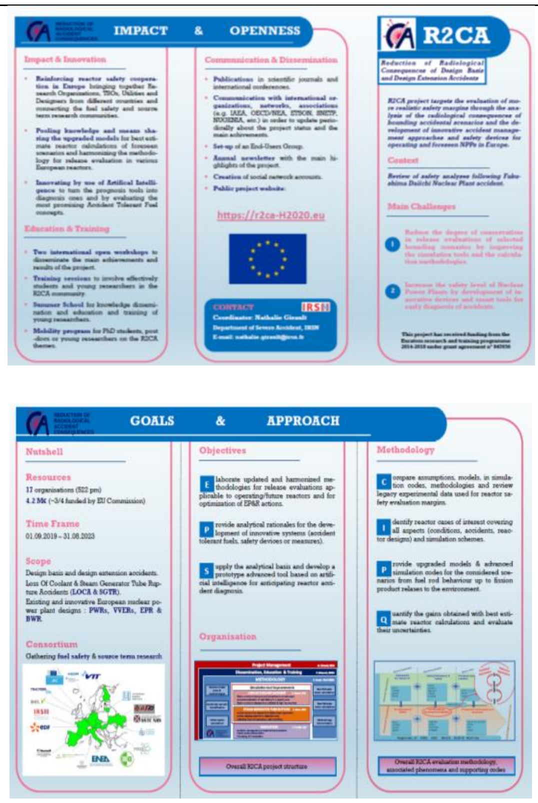


Figure 33: R2CA Brochure

Social Network accounts: An account on social media was created for communicating to the public about the project results (informing mass media about the project) and its activities (as workshops, training activities and mobility program). A LinkedIn group on R2CA and ResearchGate account has been created and all the initiative have been shared through them.

END USER GROUP

To promote the diffusion of scientific results and of the harmonized methodology developed within the project, the creation of an End Users Group (EUG) was initiated. It was open to safety authorities, technical support organizations, NPP owners, Vendors, thermal-hydraulics, fuel and source term experts, and Universities with curricula in nuclear reactor safety. The role of EUG members was to express their needs and opinions in the field of thermal-hydraulics, fuel and source term, to approach the methods developed during the project, and to exploit the project results. Three organization applied to be part of the EUG, Vattenfal (Sweden), Sapienza Università di Roma (Italy) & Politecnico di Torino (Italy) at launch. Unfortunately, due to COVID issues, the activities were stopped and not subsequently resumed, as they were too late.

MOBILITY & STUDENT TRAINING

A mobility program was set up at the project start. It intended to promote the exchange of knowledge and experience between Partners, to attract new young researchers and to enhance the availability of experts in the future for R2CA issues. Though the COVID-19 caused delays and the withdrawn of some of them (2 out of 7), several mobilities took place (**Table 3**). Several students were also involved in the project activities (**Table 4**).

Task	Duration	Home organization	Host organization	Candidate	Scientific objective
3.3	3 months	POLIMI	CIEMAT	PhD	Couple SCIANTIX with FRAPCON/FRAPTRAN
3.3	2 months	POLIMI	CIEMAT	Post-doc	Identification of developments and validation test cases for FRAPCON/FRAPTRAN* SCIANTIX
3.3	2 months	LEI	IRSN	Post-doc	Evaluation of FP release from high BU structure in LOCA with TU/MFPR-F
4.1	1-2 months	BOKU	NINE	PhD	Re-evaluation of FP transport during SGTR transient
5.1	1-2 months	BOKU	NINE	PhD	Optimisation of AMP, evaluation of measures and benefits

Table 3: Mobilities performed within the R2CA project

Task	Duration (months)	University	Candidate	Scientific objective
4.2	9	POLIMI	MSc	Include a new model for FP release in SCIANTIX (new ANS5.4) along with benchmarking
5.2	24	IRSN	Post-doc	Build & validate a fast physical model for primary circuit contamination based on detailed code results & uncertainties
5.1	36	BOKU	PhD	Investigation of iodine spike phenomena, optimisation of AMP to reduce iodine transport to the environment
2.5	12	BOKU	MSc	Validation of nodalisation approach against PSB test facility exp. for SGTR - VVER 1000 SGTR calc. up to ST evaluation
3.3	9	POLIMI	MSc	Improvement of HBS modelling in SCIANTIX
4.2	9	POLIMI	MSc	Implementation of a fuel oxidation model in SCIANTIX for defective fuel rod conditions
3.3	9	POLIMI	MSc	Benchmark between SCIANTIX & MFPR-F for HBS formation
4.2	39	POLIMI	PhD	Development and assessment of a module for gaseous and volatile FP behaviour in LWR fuel

Table 4: Msc/PhD/Post-doc performed within the R2CA project

13 Final remarks

Thanks to the developments/improvements of models, simulations tools and calculation chains in different areas (fuel thermomechanics, FP behaviour…) more realistic RC evaluations of both LOCA and SGTR scenarios within DBA and DEC-A conditions have been provided that led to reduce some conservatisms (in assumptions, model parameters…) and minimize the use of decoupling factors. The impact of new modelling was clearly evidenced through the comparison of their environmental activity releases and radiological consequences where in most cases, the improved calculations led to fewer released activities in the environment and then lower radiological consequences. and avoiding the use of decoupling factors. Datasheets for each calculation were provided which can be further use for a database creation. This represents a first step towards best estimate evaluations that should be further complemented by a more systematic study of Sensitivity Analyses and Uncertainty Quantification of what has been done during the project.

All these results and their analyses served as a sound basis for formulation of generic recommendations in Radiological Consequences evaluation for further harmonisation of their calculation methodologies. Such a harmonisation still remains challenging in a context where the choice of initial and boundary conditions of LOCA and SGTR DBA studies for example are matter of the regulation texts or agreements between the safety authorities and the Utility, in order to sustain the safety demonstration of a given NPP. These rules, often "country dependent" were not discussed during the project.

The capabilities of several different tools were also extended to study various new fuel types (as Accident Tolerant Fuels) to be used in the future (Cr-coated Zry, FeCrAl, Hastelloy-n claddings, U3Si2 fuel…), by implementing their material properties and the positive impacts of these materials on the fuel performance during LOCA conditions were assessed. These studies, for the most part, were however very preliminary and need to be complemented.

In addition, a number of modelling improvements have been made (generally more mechanistic) which could not be capitalized on in the calculation chains and/or used in the updated radiological consequence evaluations; they will be of benefit in future reactor calculations (such as internal clad secondary hydriding, FP transient releases, high burn up structure evolution and FP releases...).

Finally, exploratory work on Emergency Operating Procedures and Artificial Intelligence based tools showed that the increased capabilities of numerical tools and the use of expert methods could be advantageously used to increase the NPP safety.

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