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REDUCTION OF RADIOLOGICAL ACCIDENT CONSEQUENCES

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Abbreviations

AI	Artificial Intelligence
ATF	Accident Tolerant Fuel
BEPU	Best Estimate Plus Uncertainties
BWR	Boiling Water Reactor
DBA	Design Basis Accident
DEC-A	Design Extension Conditions-A
EOL	End-Of-Life
EPR	European Pressurised Reactor
EP&R	Emergency Preparedness and Response
FP	Fission Product
FGR	Fission Gas Release
HBS	High Burn-up Structure
IAEA	International Agency for Atomic Energy
LB	Large Break
LHGR	Linear Heat Generation Rate
LOCA	Loss Of Coolant Accident
MC	Monte Carlo
NEA	Nuclear Energy Agency
NPP	Nuclear Power Plant
PRISE	PRImary to Secondary leak accident
PWR	Pressurized Water Reactor
RC	Radiological Consequences
RCS	Reactor Coolant System
RIP	Rod Internal Pressure
SGTR	Steam Generator Tube Rupture
TH	Thermal-Hydraulics
TL	Task Leader
VVER	Vodo Vodianoï Energetitcheskyi Reactor
WPL	Work Package Leader
WP	Work Package

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1 Introduction

The main objectives of the R2CA project, dedicated to the Reduction of Radiological Consequences of Accidents with design basis and design extension conditions for Gen II, III and III+ Nuclear Power Plants, are:

- to consolidate assessments of radiological consequences of two categories of selected bounding accidental scenarios (Loss-Of-Coolant Accidents and Steam Generator Tube Rupture accidents) within the Design Basis (DBA) and Design Extension (DEC-A) domains for PWRs, EPR, BWR & VVERs;
- To propose improvements for NPP management strategies and devices to reduce the radiological consequences of these accidents.

To meet these objectives several specific actions will have to be performed:

- Make a review and collection of the existing experimental data that will be used to verify and calibrate the updated/improved models and/or advanced simulations tools developed during the project for LOCA and SGTR accidental transients ;
- Make a comparative assessment of the existing methodologies used in different countries to evaluate the radiological consequences experimental results as well as the assumptions/hypotheses, models and simulation codes that are applicable to evaluate the safety margins of the considered reactor models within DBA & DEC-A conditions, through the RC of bounding scenarios ;
- To provide advanced simulation tools and calculation schemes allowing to assess the degree of conservatism in order to be able to derive more realistic safety margins through the RC of bounding scenarios within the DBA & DEC-A domains ;
- To elaborate updated and harmonized methodologies for the evaluation and the reduction of those RC in the different kinds of operating and foreseen reactors in Europe and implemented in various code ;
- To derive from these methodologies some rationales for the optimisation of EP&R actions ;
- To provide analytical rationales for the development of innovative measures, devices and tools that could be used for the anticipated diagnosis but also for the management and mitigation of those accidents.

To this end the project is divided into four different technical Work-Packages whose specific objectives are:

- WP2-METHOD: propose harmonized methodologies for the evaluation of the RC as a marker of safety margins of both LOCA and SGTR bounding scenarios for DBA and DEC-A conditions and perform reactor case calculations
- WP3-LOCA: develop accurate evaluation tools for the evaluation of the RC of LOCA bounding 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 evaluation tools for the evaluation of the RC of SGTR bounding 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 developed evaluation tools of potential new accident management procedures/devices including Accident Tolerant Fuels but also explore the capabilities of prognosis evaluation tools to anticipate accidental configuration through Artificial Intelligence functionalities.

The calculation work performed during the 2nd project year in WP2 as well as the R&D activities carried out in WP3, WP4 and WP5 will be described in this report. In addition, will be also reported the work dedicated to the project management (WP1) as well as in WP6 regarding the dissemination/communication activities and the education/training program (e.g. the follow-up of the mobility program between different organizations in the consortium, the first training on simulation tools and the start and/or first works accomplished by PhD/post-doctoral students).

2 Work progress (WP2-METHOD, WP3-LOCA, WP4-SGTR, WP5-INNOV & WP6-DISSE)

The project was officially launched on September 2019.The first-year work was mainly focused on the preparation of the reactor calculations (selection of the accidental LOCA and SGTR scenarios of interest and some calculations had been initiated. During the second year, the calculations were completed and their result analyses performed. The tool intended for the evaluation of radiological consequences was also finalized. All of this work is included in the deliverable 2-5 in progress, which will be released very soon. Indeed, due to several problems COVID-19 related (i.e., working from home, problems connect to calculation clusters and other related workload reasons) some calculations were postponed.
Nevertheless, despite the health crisis that has been raging in Europe throughout the year 2021 and impacted the different partners of the project to varying degrees, the impact on the project (apart from WP2) has been rather limited; most of the work planned in the R&D WPs (WP3-4 & 5) could be initiated as planned in their work-plans even if sometimes with a delay. Some R&D actions have been postponed but without major consequences on the progress of the other actions and the project in general.

The main advances in the work are reported below for each of these work-package:

- **WP2**: About 48 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. For each of these scenario calculations individual technical reports have been produced by the corresponding organizations. The methodology for the evaluation of their associated radiological consequences from environmental releases was elaborated and a simplified tool provided in the form of an excel file. Finally, a first version of a dataset to collect all the calculation results was created;
- **WP3**: The test matrices for clad burst and gas axial transport were extended (e.g. the burst test database with 1350 tests). Additional tests were analysed (e.g. tests at high burn-up and on alpha radiative damages). An experimental plan for new burst tests to be performed in EK was built. Existing model reviews and, if necessary model revision/development have been started (e.g. on iodine deposition on paints, on HBS evolution, on fuel swelling by solid FP, on axial gas flow in fuel rods…). Some reviews have already been completed. Finally, an update of core plant models and of calculation schemes were also initiated;
- **WP4**: New tests on H_2 uptake by Zr4 and E110 were performed in EK. Bibliographic reviews (e.g. on secondary hydriding phenomena in defective fuel rods in normal operation conditions…) were completed. Model developments were initiated and are on-going especially regarding the phenomena related to clad secondary hydriding (e.g. gas diffusive mixing and transport in fuel rod gaps, clad hydriding, H_2 radial re-distribution, hydride precipitation…) and the iodine spiking releases under transients. Some code improvements were already done (e.g. finalisation of the TU/MFPR coupling, modification of the iodine spiking models in RING, FP releases in SCIANTIX, oxygen redistribution in fuel in TU, activity, iodine spiking release in MAAP…);
- **WP5**: The different bibliographical studies and literature survey carried out in each of the tasks of this WP have allowed an identification of the main requirements for developing advanced devices and/or accidental management procedures (e.g. algorithms for SGTR management in VVERs, an Identification of pro/cons of using Artificial Intelligence for NPP accident analyses, an analysis of existing defect diagnosis tools and AI techniques dedicated to fault detection in non-nuclear fields, and a selection of generic thermophysical/chemical properties needed for the performance evaluation of Advanced Tolerant Fuel with coated Zr clads. A preliminary concept of accident management strategy was determined for cover lift-up in VVERs and specifications for a simplified defect diagnosis tool were built;

- **WP6**: Regarding dissemination a second newsletter was issued and ten R2CA related publications were issued that were published in journals or was/will be presented in international conferences (NENE2021, NURETH19, TOPFUEL2021, Annual Meeting of the Spanish Nuclear Society, International Workshop for TU users and developers). Regarding Education & Training the first on line Training course dedicated to the open source SCIANTIX code was held gathering more than 30 participants both from institutions within and outside the R2CA consortium.

2.1 WP1-MANAG

2.1.1 Objectives

WP1 is dedicated to the overall project management. Its main objectives are to ensure an efficient scientific, administrative and financial follow-up of the project during its four year duration. Regarding the technical coordination, the WP1 will that all the produced scientific work will be implemented in compliance with the quality standards and with respect to the planned time schedules, delivery tables and budget. It will also verify that the produced work meet the project main and specific objectives.
During the second year, the main challenge of the management team was to keep the link with the different actors of the project by continuing to promote the interactions between the partners and to favour the collaborative performance of the activities in agreement with the established work-plans.

2.1.2 Overview of the main advances

The first year progress meeting was held remotely, gathering more than 50 European experts, researchers and students from the 17 organisations participating to the project, in October 2020. During this meeting the main first progress in the project work were presented and discussed. It mainly concerned the different reviews carried out on release evaluation methodologies, on simulation tools/calculation schemes and on experimental database as well as the preliminary reactor calculations results dedicated to LOCA and SGTR accidental scenarios. The future steps for the forthcoming year in the R&D WP3, WP4 and WP5 were also discussed and the work plan established for each of the organizations involved during the three years of their duration were presented.

During this first year the first Steering Committee and first Management Team meetings were also organised respectively in November 2020 and April 2021. During these meetings were respectively discussed:

- The Data Management plan and more especially the open-access publication strategy to be agreed on; the possibility of redistributing part of the budget, initially allocated to travels and which was saved because of the health crisis, for the financing of mobility and/or PhD/post-doctoral students. A discussion was also held on LOCA reactor calculation strategy where in several calculations the peak cladding temperatures predicted by the codes are not high enough to lead to clad failures and therefore to the release of fission products. Finally the composition of the Advisory Panel Group scheduled to meet along the 1st Open Workshop that will be organised in 2022 was also debated and several experts proposed.
- The status of the work and the main progress made in each task of the WP3, WP4 and WP5 since July 2020 (official start of the R&D activities in these WPs). Main outcomes of the reactor test case simulations were also debated as well as the calculation data sheets to be elaborated.

Finally the consortium agreement was also agreed amongst partners and signed.

2.2 WP2-METHOD

2.2.1 Objectives

The main objectives of WP2 are:

- Propose harmonized methods for evaluation of the radiological consequences of both SGTR and LOCA categories of DBA and DEC-A accidents;
- Perform best estimate evaluations of reactor case configurations for PWRs, BWRs, VVERs and EPR by using improved calculation schemes;
- Analyse the potentiality of accident management measures and devices, including innovative actions to reduce the radiological consequences of those accidents.

The work-package is subdivided into 8 tasks. Amongst them the three first tasks dedicated to review of release evaluation methodologies, simulation tools and available experimental database relevant for the development/validation of models dealing with LOCA and SGTR phenomena were already completed at the end of the first year. Reactor scenarios of interest to be calculated within the project were also selected.

The WP2 work during this second year of the project focussed on the first set of reactor calculations (including the development of a simplified tool for the evaluation of the radiological consequences from FP releases) and on the main uncertainties identification for the releases evaluation. The specific objectives of the corresponding tasks (task 2.2, task 2.3 and task 2.4) for the time period considered are recalled below:

- Task 2.2 – The objective for this task was:
  - Propose simple methodology for the evaluation of the radiological consequences from a given environmental source term.
- Task 2.3 – The objectives for this task were
  - Make a first set of simulation of the reactor cases determined in task 2.2 that will be used as a starting point in task 2.5
  - Analyse the calculation results
- Task 2.4 - The objective for this task was:
  - To understand and get insight in the uncertainties in the reactor case calculations performed in task 2.3. by qualitative description of the different sources of uncertainty
  - Propose a global approach for evaluating the uncertainties in the calculation methodology

2.2.2 Overview of the main advances

For task 2.2 a simple methodology and the corresponding excel file for the evaluation of the radiological consequences from a given environmental activity was built. This model is implemented in Microsoft Excel and is able to convert the released activity at the release point into a dose received by a person at a certain distance.

Task 2.3, which consists of a simulation of the scenarios presented in task 2.2, has been completed. About 38 individual technical reports have been released by each organisation involved in the calculations for LOCA DBA, LOCA DEC-A, SGTR DBA and SGTR DEC-A conditions. The deliverable summarizing the calculations results and highlighting both the model development needs for a more realistic evaluation of the source term and model improvements that will be performed within the project is under completion.

A datasheet was also proposed to gather the overall calculation results that will serve at the end of the project to develop a database.

Finally, in Task 2.4 a draft of the deliverable addressing the Uncertainty Analyses was elaborated including specific tables where the evaluation of the relevant actions & phenomena for uncertainty related to the scenario case studied within the project was done and a global uncertainty approach in the case of code coupling was proposed.

2.2.3 Details of the activities performed

2.2.3.1 Task 2.2: Scenario identification & radiological evaluation tool

Last year it had already been decided that all partners would use their own model/configuration. Additionally the first steps toward a simple tool for the calculation of radiological consequences was performed.
The tool consists out of a simple Excel file which implements a simple model for the calculation of radiological consequences. The proposed model consist out of two parts. One part which models the dispersion in function of the height of the release point, the distance release point -receiver and the stability class of the ambient air. For the dispersion model a Bi-Gaussian Plume model is used with Briggs-equation to model the behaviour of the ambient air.
A second part transforms the activity received into a dose expressed in Sievert (6 different age categories are considered). Therefore certain contributions are not taken into account (e.g. no consequences of intake are taken into account) and the calculations are focussed on to the event effective dose (due to inhalation & external exposure) and the equivalent thyroid dose. The different formulas which are used originate from the different ICRP guides (e.g. breathing rate is based on CRP 71).

2.2.3.2 Task 2.3: Initial set of reactor calculations

During the second year of the project, two video-conferences were organized (on February 2nd, and February 10th of 2021) for the LOCA and for the SGTR accidents. The main purpose of these meetings was to share and discuss the reactor test case simulation results received by the different partners involved in this task. In addition the main observations issued from these calculation results were highlighted and encountered problems discussed. Finally, the concept of the datasheets for the collection and harmonization of the data and results of all these calculations (which will be used in the final preparation of the database) was also discussed as well as the content of the deliverable D2.5 summarizing all this work.
During the 2nd year, the different partners of the R2CA project worked on their modelling methods, calculation schemes and used different modelling tools in the framework of task 2.3. A list of the initial reactor test case simulations performed within the project is presented in Table 1. At the current moment, all planned calculations and the analysis of their results have been performed. In addition, individual reports have been written for each reactor accidental case and uploaded in the project share point. Only exception, IRSN do not perform SGTR accident analysis under DEC-A conditions. This analysis will potentially be performed in the frame of task 2.5.
Draft report of deliverable D2.5 is prepared, but still need to be circulated amongst the partners in order to confirm presented data and the analyses of the results is on-going. As expected due to difference in reactor model technology and in the assumptions for initial and boundary conditions the results in terms of released activity significantly differs from one calculation to another. A more detailed analysis of the results is in progress to explain the most divergent results which are few.
Deliverable D2.5 where the main outcomes of these calculations, the modelling methods and approaches as well as the main hypotheses and assumptions used will be given is planned to be finished in two months.

Table 1: Initial reactor test case simulations performed within the project

Organization	Type of reactor	LOCA		SGTR	
		DBA	DEC-A	DBA	DEC-A
ARB	VVER-440; VVER-1000	Performed; Performed	Performed; Performed	Performed; Performed	Performed; Performed
Bel V	PWR-1000	-	-	Performed	Performed
BOKU	PWR-1300, VVER-1000	-	-	Performed; Performed	Performed; Performed
CIEMAT	PWR-1000	-	-	Performed	Performed
ENEA	PWR-900	Performed	Performed	-	-
HZDR	PWR-Konvoi	Performed	Performed	-	-
IRSN	PWR-900	Performed	Performed	Performed	Cancelled
LEI	BWR-4	-	Performed	-	-
EK	VVER-440	Performed	-	Performed	-
SSTC-NRS	VVER-1000	Performed	Performed	Performed	Performed
TRACTEBEL	PWR-1000	-	-	Performed	Performed
UJV-NRI	VVER-1000	Performed	-	Performed	-
VTT	EPR-1600; VVER-1000	Performed	-	-	-
		-	Performed	-	-

Finally, a template for datasheets was prepared to be completed by each partner with their calculation data and results. The main purpose to these datasheets is to have partner's results in a numerical format to ease the comparison at the end of the project between initial and final calculations and thus highlight the progress made in the calculation methodology and model improvements.

2.2.3.3 Task 2.4: Uncertainty evaluation

The deliverable of the task has been completed in a draft version and has been send to the Task 2.4 partners for internal review. It is now ready for a review of all the other project partners.
The report includes these main aspects:

- Description of the general framework of the project, description of the task and role in the project.
- Uncertainty sources - The main sources of the uncertainty are identified. The analysis of the uncertainty sources is performed at a qualitative level. The goal is to point out the aspects to be included in the uncertainty analysis.
- Uncertainty relevance of phenomena/actions for the considered scenarios: LBLOCA and SGTR (DBA and DEC) - Among all the uncertainty sources the relevant sources are identified and are ranked based on their impact for the considered scenarios.
- Overview of uncertainty evaluation approaches - This is an overview of the approaches developed to evaluate the uncertainty. The description is done at a qualitative level.
- Proposal for global uncertainty approach. An approach to evaluate the global uncertainty in the case of coupled codes is proposed. The global uncertainty is due to the combination of the linked codes uncertainty.

2.3 WP3-LOCA

2.2.1 Objectives

This Work Package aims to improve the different simulation tools and models used to analyse to the LOCA transients and to evaluate the corresponding releases. It will focus on modelling fuel rod cladding failure and calculating the quantity of failed cladding in the reactor core, evaluating releases of fission products into the RCS and their transport to the environment.
It is planned to develop the knowledge and the accurate evaluation tools dealing with the evaluation of the radiological consequences of loss of coolant conditions for bounding scenarios of both DBA and DEC-A domains. To that extent, existing databases and models will be revisited and existing codes will be enriched and adapted. Code improvements will be on both accident progression and source term up to the environment related phenomena.

The work-package is subdivided into 3 tasks respectively dedicated to:

- Task 3.1: Fission product transport and release from the primary circuit to the environment (lead UJV)
- Task 3.2: Evaluation of failed rod number (lead IRSN)
- Task 3.3 Fuel rod behaviour during LOCA transient (lead JRC).

2.2.2 Overview of the main advances

The main progresses made during the second year of the project are briefly described below:

- Regarding the fission product transport and release, it has been performed a bibliographic review regarding ELSA, that models the fission products and structural material release and also a study with ASTEC/ELSA is ongoing for the simulation of Cs release. It has been conducted a revision of iodine behaviour models in COCOSYS. Several hundreds of calculations were performed, which led to determination of a new set of adsorption and desorption rates as well as an updated value of splitting factor between physisorption and chemisorption.
- Regarding the evaluation of failed rod, Best Estimate models were adjusted on the basis of the experimental database built previously in the project. It has also been undertook the re-assessment of burst failure criteria in order to decrease the scatter of the measured data. Some improvements have been made: M5 model, plastic deformation model of the code FRAPTRAN. DRACCAR, ATHLET-CD and ASTEC capabilities are extended to the description of a whole core. These works are ongoing. Some contributions were dedicated to statistical methodology for the determination of the evaluation of the quantity of the fuel rod failures: (RELAP or ATHLET) with the TRANSURANUS; FRAPTRAN.
- Regarding the fuel behavior during LOCA transient, it has been performed a coupling of the TRANSURANUS fuel performance code with the mechanistic chemistry code MFPR-F and the 0D grain-scale code SCIANTIX, tailored for fission gas behavior modelling. SCIANTIX has been improved also regarding High Burnup Structure (HBS) modelling.

2.2.3 Details of the activities performed

2.2.3.1 Task 3.1: Fission product transport and releases from primary circuit to environment

The main objective of the task 3.1 for the second year was to improve the code abilities. Only UJV and ENEA conducted work in this field. Other partners expect to start the work in the second half of 2021 or in the beginning of 2022. No delay is expected.
In the framework of the WP3.1, ENEA is involved in the revision of the ASTEC capabilities in modelling the FP release; in particular, ENEA has performed a bibliographic review regarding ELSA, which is the ASTEC module that models the fission products and structural material release during core degradation.
Based on the validation matrix reported by Cantrel et al., the data having the conditions of interest for this project are very limited. Only the VERCORS experimental program includes very high-BU fuel tests but they are run at high temperatures; some data are available at lower temperatures (plateaus at 800°C and 1000°C) but the BU is not very high. Phebus FP has low temperature data but, also in this case, the BU is quite low.
According to Brillant et al., the release models do not consider the BU effect on the FP release, causing some discrepancies in high BU validation cases; for this reason the authors suggest that high BU UO_2 models should be developed in the future.
The review also reviewed the R2CA experimental database, established in the T2.1.3 of the project and documented in the deliverable R2CA D2.3 by Hozer et al., for potentially useful data to extend ELSA validation in the considered conditions: in particular ACCR-ST, FLASH-LOCA, GASPARD and VERDON experiments can be interesting in this framework.
In addition, a study with ASTEC/ELSA is ongoing for the simulation of Cs release in VERCORS RT1 and RT6 experiments, characterized by similar thermal-hydraulic conditions and different BU. The main objective is to analyse if, in absence of a specific model, the effect of BU can be artificially caught by ELSA through the optimization of the input parameters dealing with the fuel grain size distribution.
The optimization study is planned to be performed using RAVEN tool coupled with ASTEC. As an alternative, the parameters related to grain size distribution will be optimized by using a more classical approach based on ASTEC parametric studies.

In the frame of the task 3.1 UJV conducted a revision of iodine behaviour models in COCOSYS. Regarding the experimental database created within the task 2.1.3. and the investigation conducted, phenomena for further improvement was selected. This led to further investigation of the iodine dry paint deposition model in COCOSYS with utilization of data from the OECD NEA BIP (Behaviour of Iodine Project) experimental programme, namely the IA (Iodine Adsorption) experimental series. The data in this series included several experiments conducted with the Ameron Amerlock paint, which is present in the Temelin NPP as a containment steel liner coating. Initial calculations of the experiments revealed several disagreements between experimental and calculated values. In general, adsorption as well as desorption was underestimated. Furthermore, the ratio between physisorbed and chemisorbed iodine was not calculated correctly. This inconsistency was expected, because the basic model setup is derived from the behaviour of GEHOPON paint from Arndt et al., which is often used on German NPPs. Following effort comprised several hundreds of calculations, which led to determination of a new set of adsorption and desorption rates as well as an updated value of splitting factor between physisorption and chemisorption. This work was summarized and presented at the NENE 2021 conference in Bled, Slovenia. Further work should comprise an impact of this improvement on the iodine released mass during LOCA.

Other partners involved in this task (i.e. HZDR, IRSN, SSTC, VTT) have not yet started their work.

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2.2.3.2 Task 3.2: Evaluation of failed rod number

The main objective of this task is to better evaluate the number of failed rods during a LOCA. Partner’s contributions to task 3-2 during the 2nd year were related to:

- Cladding burst:
  - LOCA burst database (IRSN)
  - Reassessment burst models and propose new burst criteria (IRSN, VTT, EK)
  - Development thermo mechanical (phase transition, creep) models for M5 (ENEA)
- New core modelling:
  - Parametric studies and impact of relative power in rings with ASTEC (LEI)
  - Development of a new code chain (DYNS3D + RELAP/TRANSURANUS) (SSTC)
  - Development of new core modelling/meshing with DRACCAR (IRSN)
  - Development of new core modelling with ATHLET-CD (HZDR)
- Statistical methodology:
  - Proposal of a new code calculation chain for statistical analysis (VTT)
  - Development of UA and SA tools for TRANSURANUS (JRC)
  - Development of a statistical methodology to be used with TRANSURANUS (UJV)

IRSN work during last year was dedicated to burst criteria definition and DRACCAR new modelling for whole core simulations.

More than 1400 burst tests from about 20 experimental programs were collected, most of the tests were run on Zy-4 cladding under temperature ramp tests. Historical burst criteria (Nureg-630 strain upper limit, Chapman model on engineering stress, EDGAR Zy-4 creep criteria) were compared to the new burst database. Best Estimate Chapman type models on engineering and true burst stresses as well as exponential models with and without the impact of the heating rate were adjusted. Finally, different exponential models were adjusted in order to obtain minimum, maximum, mean, mean ± std correlations on true burst stress. These correlations can then be used for sensitivity analysis to evaluate the number of failed rods during a LOCA.

The DRACCAR multi-rod and multi-physics code at the assembly scale dedicated to LOCA is based on a coupling between 2.5D multi-rods thermal-mechanical modelling and a 3D thermal-hydraulic description at sub-channel scale. DRACCAR is able to model fuel assembly behavior under LOCA conditions by coupling rod deformation to flow blockage. However DRACCAR is currently not able to depict a whole core - except by using a standard approach based on averaged weighted rods which cannot lead to a detailed evaluation of the rod failure number. In the frame of R2CA, DRACCAR capabilities will be extended to the description of the whole core coupled to reactor primary and secondary loops. This approach will mix modelling scales with fined assembly description at sub-channel scale as well as coarser meshing using lumped volume and equivalent weighted rods to depict other parts of the core. Both scales will be managed in a single simulation proposing the whole core response to a LOCA. The first part of the DRACCAR work plan is in progress. Several preliminary studies preparing the development of the new modelling scheme have been realized. These studies are based on cases using either 3D meshed rods (basically an eighth of a fuel assembly) or weighted equivalent rods. The modelling mainly consists in fuel assembly modelling within a DRACCAR domain coupled to thermal-hydraulic boundary conditions (from system thermal-hydraulic studies). The preliminary conclusions deduced from this studies highlight that: within a fuel assembly, the rod responses (creep and potential burst) are influenced by the distance to guide tubes (cold spot) and by the local rod power whereas the classical equivalent rod approach is not able to account for this. Moreover, for high burn-up MO_X fuel assembly, Pu enrichment varies within an assembly and significantly influences the rod internal pressure (mainly due to helium production during irradiation phase). Rod initial pressure is a key parameter to evaluate ballooning and burst. This preliminary work tends to conclude that within a fuel assembly, in some configurations (depending on LOCA transient and FA design and irradiation state), the scattering of rod behaviors should be taken into account to estimate precisely the number of rod failures during LOCA.

The equivalent rod model was improved. Indeed, the ballooning of the equivalent rods is now limited to the rod pitch and the evaluation of contact surface ratio allows to decrease the heat exchanges surface with the fluid. Another important new DRACCAR feature is the initialization of DRACCAR fuel rod initial conditions by extracting FRAPCON4.0 irradiation simulation results to the DRACCAR input deck. This feature seems necessary for the future whole core application. Finally, a corrective factor applied to burst strain criterion and deduced from REBEKA outcome was implemented to reduce burst strain with respect to azimuthal temperature difference (which can be evaluated using DRACCAR 3D simulations).

This first phase is pursued by the analysis of the interactions between a fuel assembly and its neighbors during a LOCA. The investigations on modelling using mixed meshing involving several weighted equivalent rods and 3D fined meshed rods are going on. It should lead to propose new core applications able to take into account more in depth the behavior of some fuel assemblies and their interaction with the rest of the core. In a last step, the core domain will be included in a whole reactor circuit simulation (RPV, primary and secondary loops). It's expected that this method will be valuable to improve the rod failure prediction capabilities.

ENEA, during the second year of the project, has undertaken a review on two physical properties of the M5 alloy: the crystallographic phase transition and the high temperature creep. With regard to phase transition, two models have been considered: Massih (2009), and Massih & Jernkvist (2021). A model based on a Leblond & Devaux (1984) equation has been proposed for M5 that could be capable of accounting for heating rates up to 100 °C/s and concentrations of hydrogen up to 100 ppm. Concerning the high temperature creep, three models have been compared: Kaddour et al. (2004), Trego (2011), Massih (2013). The analysis conducted on these models has been mostly focused on the behaviour of creep in the (α+β) domain where the increase of β grains size plays a significant role. This work should provide an adequate source of information to move towards the introduction of new correlations in the TRANSURANUS code and a validation of M5 models based on the simulation of specific LOCA tests. Planned work should be accomplished timely during last year of the activity.

In WP 3.2, EK undertook the re-assessment of burst failure criteria 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 is to study the geometry of samples of the Russian alloy E110 that underwent ballooning and burst tests. In the second phase new burst criteria are to be established. Finally in the third phase, using these new criteria the parameters of the cladding plastic deformation model of the code FRAPTRAN are to be re-fitted.

In order to measure the geometries of ballooned and burst samples, a Keyence VR-5100 Wide-Area 3D Measurement System has been procured at EK. The methodology to measure the outer and inner diameters of entire samples as a function of the axial and circumferential position is under development and testing. In the meantime the thickness of a set of E110 samples produced earlier, filled with acrylic resin and cut at mid-burst position, is being measured as a function of the circumferential position to assess the reasons for the scatter of the strain data. The new burst criteria can be established based on the detailed geometries to be measured in the next step.

Re-fitting the FRAPTRAN cladding plastic deformation model is an iterative process based on the Levenberg-Marquardt method, where in each iteration step the actual values of the model parameters are input to the code and the code output is compared to the measurements. The programs necessary to do this fitting were developed during this work period, the fitting runs can be started once the new burst criteria are available.

HZDR work during the 2nd year was dedicated to the development of a detailed core model in ATHLET-CD (part of the AC² code package). A new core modelling approach for ATHLET-CD is currently developed by code owner GRS, Lovasz et al. (2018), Wielenberg et al. (2019). GRS provided a beta-version of the code to HZDR for testing and first application of the new model. There are two new approaches for modelling of the core, Weber et al. (2019): The first is based on a subdivision of the radially concentric core rings (original ATHLET-CD approach) into several azimuthal segments. That approach was tested first. The input data set applied in Task 2.3 (reactor calculations) was modified: The originally implemented six concentric rings were subdivided into 8 segments per ring. Furthermore, one additional section is introduced which represents the central fuel assembly (in total 49 core sections). However, that approach has the disadvantage that each core section represents several fuel assemblies and the power distribution had be averaged within each section.
The second approach offers the possibility to sub-divide the core into a user-defined number of sections located within an x-y-coordinate system. The approach was originally developed to model accidents in spent fuel pools (SFP), which could not be described by the original concentric ring approach of ATHLET-CD. The applied subdivision for SFP was in the order of 6-25 sections, Lovasz et al. (2018), Weber et al. (2019). To model a Konvoi PWR on assembly level, a much larger number of sections is needed (a 15 by 15 matrix with in total 193 active core sections + 32 dummy sections at the corners). Compared to the original approach (applied in Task 2.3) with six concentric core sections, that model is significantly more detailed. Each section contains one representative fuel rod that represents 300 fuel rods (= 1/193 ≈ 0.52 % of the total number of fuel rods). Based on the number of core sections, which fail during the transient, the percentage of failed rods could be estimated in steps of 0.5%. In general, a further sub-division of the core sections seems to be possible, e.g., a 9x9 subdivision of each fuel assembly, resulting in 1737 active core sections. The fuel rods of one assembly can be grouped by power and/or burn-up to estimate the conditions for each of the smaller core sections. By that approach, the highest-power rods could be assessed separately.
To model the radiation between the core sections, view factors are calculated by ATHLET-CD between each surface of a core section (axially sub-divided) and all other surfaces of all other core sections. That results in a huge number of view factors and not sufficient memory in available computers. As radiation is of negligible importance in the low temperature range (< 1200 °C), it was decided to switch off the radiation calculation in the source code. Further improvements were implemented in the code to handle the increased number of control volumes and parameters written to ATHLET-CD plot files, and to speed up the simulations by run-time profiling. With these improvements, it is now possible to simulate a 300-s-transient of LB-LOCA within approx. 40 hours run time on a single CPU.
The (realistic) core power distribution has been extracted from a pin power file of a generic German PWR (Konvoi type with 18x18-24-fuel-rod assemblies) for different core-states of a generic equilibrium cycle (ranging from 0.0 to 330.0 equivalent full power days). A Python script has been developed to map the power distribution to the ATHLET-CD input file (average power factor per assembly + average axial profile).
The first analyses with the model have shown that considering realistic power distribution and fuel rod parameters, rupture of the rods in DBA-LBLOCA scenario is very unlikely. One reason is the relatively low fill gas pressure of Konvoi fuel rods (2.25 MPa, Wunderlich et al. (1990)), which is close to the lower boundary of the typical range for PWR, EPRI (2013). RIP increases with increasing burn-up, and the estimated cold-state pressure at EOL (60 GWd/MTU) is approx. 3.6 MPa (based on formula given in EPRI (2013), significantly lower than RIP for other fuel types. The max. (best estimate) linear heat generation rate (LHGR) is approx. 350 W/cm (at beginning of cycle), which leads to relatively low peak cladding temperature of 650 °C during the first peak ("blowdown phase"). Furthermore, coolant is injected by safety injection systems (accumulators, high-pressure safety injection pumps and low-pressure residual heat removal pumps) from both sides (from cold legs and from hot legs). That combined injection is a Konvoi specific design feature, which leads to efficient reflooding and fast cool-down of the hot region at the top of the core. Therefore, for Konvoi PWR, the second temperature peak ("reflood phase") observed during a DBA-LBLOCA is usually lower than the first peak, Kozmenkov&Rohde (2013). That further reduces the risk of cladding tube rupture.
As a next step, in order to reach rupture of fuel rods, conservative conditions were applied. The assembly power factors are still based on the realistic power distribution, but combined with a top-skewed power profile (max. LHGR = 465 W/cm). Furthermore, 106% of nominal reactor power and high rod internal pressure (RIP = 3.06 MPa at cold

state) were applied. Under these hypothetic conditions, rupture of rods is observed for high-power rods. The evaluation of these results is still in progress.
One issue in the ATHLET-CD code is that initial RIP can be defined in the input only as a single value, which is applied to all core sections. As RIP is burn-up dependent, that simplification should be removed. It is planned to modify the source code such that the cold-state RIP can be defined separately for each core section (as a function of burn-up, e.g. by the correlation RIP (in MPa) = 2.25 + 0.0224 * BU, based on EPRI report (2013), but with lower initial value at BU = 0. A detailed investigation of RIP will be performed by additional analyses with TRANSURANUS.

In JRC, the statistical post-processing program TUPython of the TRANSURANUS package was further improved in order to support the Best Estimate Plus Uncertainty (BEPU) analyses. Thanks to the Monte Carlo input sampling approach, uncertainties of up to 40 safety-relevant modelling variables can be statistically estimated. In a paper submitted to TOPFUEL2021 conference to be held in Santander, Spain from 24-27 October 2021, the main functionalities of this tool were outlined and illustrated using a test case and a numerical experiment based on Wilks' formula. More precisely, we illustrated how the standard statistics can be calculated with the new graphical user interface and demonstrated a numerical experiment with 1st to 6th order Wilks' methods. Based on the numerical experiment we showed that the 1st order Wilks' method for calculating the 0.95/95% uncertainty estimator contains also uncertainty in itself and can deliver very conservative values for a safety-relevant variable.

In LEI, according to the prepared plan for the T3.2 it was planned to make new ASTEC nodalization for the core region of BWR-4 and update input deck. It was planned to increase number of concentric rings, change axial and radial nodalization. However, it was decided to move to a different direction – to change only the relative power of the existing concentric rings. For this methodology, the separate concentric rings of the core region were modified keeping the same relative power of the whole core. Using this methodology, it is possible to find at which power of the concentric rings cladding burst is achieved under analysed LOCA scenario. Specific loading map of reactor core were assumed in the T2.3. This methodology enabled more precisely to distinguish number of damaged claddings. Changes in the power of the concentric rings should be related with the flow rate through this ring. This was taken into account for the provided modification. Applied methodology showed that ~42% of claddings from all core region will be damaged in the case of DEC-A LOCA. Previous results showed ~55% of core region damage (cladding burst). In the future it is planned to make new nodalization scheme of core region and to use TRANSURANUS code for the more detail analysis of the processes in fuel during LOCA.
In the frame of this task a parametric analysis of the ASTEC code were performed. Sensitivity of oxidation parameters: zirconium oxidation physical laws (Cathart, Urbanic, Prater), start of oxidation temperature, maximal hoop strain allowed before burst and axial extension of the cracking after clad burst was analysed. This was done to investigate parameters that influence the cladding burst time, total hydrogen generation and fission product release. The analysed parameters showed small effect to the cladding burst time (time difference less than 10 s). However, it showed significant influence by increasing hydrogen generation and the fission product release.
Results of this analysis will be used for the development of updated model for DEC-A LOCA analysis in the frame of T2.5.
Currently the development of the BWR fuel rod model for TRANSURANUS code started. Initial parameters and boundary conditions will be taken from the ASTEC calculation results. First results are expected at the end of the year.

At SSTC-NRS a multistage approach of evaluation of the failed rod number for a VVER 1000 LB LOCA is used. It consists of preliminary preparation initial data for LOCA by fuel behaviour history simulation and further chain calculations with use TH code RELAP and TRANSURANUS with respect to evaluation of failed rod.
To simulate the behaviour of a fuel rod in a LOCA accident using the TRANSRANUS code, it is necessary to determine the boundary conditions in the form of the external temperature of the fuel rod zirconium cladding. For this purpose:

- VVER-1000 core DYN3D model for simulation fuel power behaviour history has been developed to elaborate representative VVER-1000 core with Russian design fuel assembly TWSA. The prepared data consist of consequent four fuel cycles to simulate pin-by-pin initial parameters with whole burn-up history before start of LOCA initial event;

- TRANSURANUS models for VVER fuel pins behaviour analysis have been developed;
- Fuel power/behaviour history has been simulated by calculating proposed 4 VVER-1000 fuel cycles to prepare fuel pin initial data for LOCA with use of the developed DYN3D and TRANSURANUS models.

The boundary conditions in the form of the external temperature of the fuel rod zirconium cladding should be determined to simulate the behaviour of a fuel rod in a LOCA accident using the TRANSRANUS code. For this purpose from the fuel power/behaviour history simulation 5 fuel rods with different power/burn-up were selected for further LOCA calculation using the RELAP code. Fuel pins power (Kr) and height profiles for 5 fuel elements for the RELAP code were selected for the representative Kr range 1.36 ... 1.00 (the minimum in the core is ≈0.2). The end of cycle (EOC) moment of the cycle was chosen as representative.

UJV work last year was dedicated to the finalisation of the statistical methodology for the determination of the evaluation of the quantity of the fuel rod failures. The methodology is based on loose coupling of a system code (RELAP or ATHLET) with the TRANSURANUS fuel performance code. The aim of this methodology is to focus on the pre-LOCA rod internal pressure as a driving force for the ballooning and burst.
The system code provides the fuel performance code with the history of the pressure in the core, heat transfer coefficient from coolant to cladding, liquid and vapour temperatures and vapour fraction. These are provided either for a hot channel (conservative option) or for a number of channels corresponding to different fuel assembly powers. These data are used to define the LOCA specific part of the TRANSURANUS input.
The statistical analysis in the TRANSURANUS code considers the uncertainties in the

- Fuel rod as fabricated parameters
- Code models and material properties

A suite of scripts for sampling from the selected range of values, input preparation, code execution and evaluation of the results was prepared.
Selected number (typically 100) of TRANSURANUS runs is performed, each case is defined by

- rod power history and burn-up (in a current, conservative, approach a bounding power history is used for the pre-loca burn-up and hence the power history is determined by the burn-up, but for a realistic calculations core specific data are used)
- pre-LOCA rod power and axial power profile

The outcome of the statistical calculations is the determination of rod states, which lead to clad failure for the considered LOCA scenario defined by “pre-LOCA rod power and rod burn-up”. By mapping these states on the rod distribution in the core, the number of the failed rods is obtained.
The advantage of this approach is the variable level of conservatism, determined by the level of detail of the system code boundary conditions (single hot assembly in the most conservative, multiple channels in detailed core model in realistic). The disadvantage is the loose (one-way) coupling between fuel rod and system calculation.

VTT’s work for the second project year concentrated on improvements on the calculation chain for LOCA simulations. The general outline of the statistical system developed previously for the purpose of EPR LB-LOCA analysis has been maintained, with FRAPTRAN-GENFLO and FRAPCON used for fuel behaviour analysis and Apros for system modelling. The feasibility has now been demonstrated also for VVER-1000. The chain of simulations codes was modified by replacing CASMO with Serpent in generation of cross section libraries for Apros. This change facilitates the use of new software tools developed within VTT’s new reactor simulation framework called Kraken. GRS’s SUSA uncertainty and sensitivity analysis software was replaced by in-house sampling tools that make use of open source scripts. Demonstration of the sampling has been done in Task 2.3 by sampling local parameter values in fuel behaviour simulations of all the rods in VVER-1000 reactor. The system code Apros model for VVER-1000 was updated to Apros 6.10 environment by revising the RPV nodalization and heat structures, adjusting logics and several safety and auxiliary systems. The model was originally built in 2007 in Apros 5.07 environment and validated against a steam header break transient, and in 2015 the model had been updated and modified for the V1000-CT benchmark.

As a next step, cladding failure models will be updated in FRAPTRAN and the EPR simulations will be repeated with the updated models. No cladding failures were detected in VVER-1000 simulations according to FRAPTRAN, and therefore those simulations will not be repeated.

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2.2.3.3 Task 3.3: Fuel rod behaviour during LOCA

The main objectives of the second year were to finalize the re-assessment of the experimental database for fuel rod behaviour based on the IFPE database at OECD/NEA by adding complementary tests of interest for the validation of the models that will be developed within the project (i.e. on the impact of power cycling or HBS on radionuclide releases), develop/revise models in codes (i.e. description of the HBS, fission product releases, gas transport in the fuel rod gap and clad large deformation) and carry out the couplings between fuel thermo-mechanical behavior codes and mechanistic tools simulating the behavior of fission gases and the release of fission products at grain scale.
The JRC has been working closely with IRSN and POLIMI on a refined two-way coupling of the TRANSURANUS fuel performance code with the mechanistic chemistry code MFPR-F and the 0D grain-scale code SCIANTIX, tailored for fission gas behavior modelling. Either of these two mesoscale codes can be called as point model for each fine zone of the Transuranus nodalization. In addition to a detailed evaluation of the local concentrations of fission products, the local swelling strain is simulated by either MFPR-F or SCIANTIX and fed back to the total strain calculation by TRANSURANUS. Both SCIANTIX and MFPR-F are implemented as an optional plug-in to TRANSURANUS (i.e. replacing a dedicated blind interface) that can be provided to the user if licensing conditions are fulfilled with respect to POLIMI and IRSN.

This code configuration now allows the LOCA experiments Ifa 650.10 (PWR) and Ifa 650.11 (WWER) to be simulated with different approaches for fission gas behaviour, i.e. the TRANSURANUS empirical and mechanistic models, as well as the mechanistic chemistry model of MFPR-F and an interim version of SCIANTIX (for base irradiation so far). The different modelling approaches lead to considerable variations in both kinetics and level of total fission gas release, already in the base irradiation. Further analysis is required, as the total amount of fission gas must be carefully accounted for later evaluating the eventual release of radioactive fission products (to be addressed in WP4). As expected, there is however only negligible impact on the time of cladding burst and the final cladding deformation. Recent calculations with the latest TRANSURANUS version have confirmed the fair agreement with experimental data and are consistent with earlier results from the IAEA FUMAC project.

At IRSN, one high-burnup test (NRC Studsvik 192) has been further analysed using TRANSURANUS/MFPR-F in coupled mode. The irradiation of the father rod showed that restructuration of the UO_2 crystal occurs at the rim of the pellet, over a zone of 400 micrometres, in fair agreement with literature data. The fission gas contained in this HBS zone represents 12% of the total FG inventory. Restructuration is also observed in the internal part of the pellet. Further investigation of the microstructure evolution under irradiation showed that episodes of strong nucleation of dislocations occur during the power ramp at the beginning of irradiation cycles, increasing significantly the dislocation density. These episodes play a major role in the fuel restructuration, but their physical relevance still has to be investigated, especially for the pellet centre. The LOCA transient has then been simulated using the restart capability of the coupling. The time of burst and final cladding deformation were in good agreement with the experimental data. No fission gas release was obtained in the simulation, which is due to the fact that the model of MFPR-F for FG release from HBS is not yet activated in the coupling. Its activation is foreseen in the work plan of IRSN, along with its improvement in the framework of the coupling with TRANSURANUS, which allows to take into account the effect of clad restrain. As an additional topic, the work on FP release induced by fuel oxidation by steam after clad burst will be started. This topic will be studied at the pellet scale with stand-alone MFPR-F in multi-mesh mode, which includes a model for pellet surface oxidation and oxygen redistribution in the pellet. In parallel, a simplified model of fuel oxidation will be proposed for MFPR-F in point mode, applicable in the context of the coupling with TRANSURANS, and its results will be compared to those obtained with standalone MFPR-F.
The coupling system of the meso-scale SCIANTIX open-source code (POLIMI) and TRANSURANUS is being updated and extended. Current work focuses on the restart capabilities that is essential for simulating refabricated fuel segments in a research reactor after base irradiation, e.g. in a commercial nuclear power plant, and should allow for an extended analysis of the above mentioned LOCA simulations. First results have been presented at the online workshop "Towards nuclear fuel modelling in the various reactor types across Europe" organised by JRC for the TRANSURANUS users 28-30 June 2021. As the TRANSURANUS code includes modelling extensions developed in further European projects (e.g. INSPYRE, MacSafer), all simulations are verified with the most recent code version (v1m5j21).
POLIMI has made further progress in the modelling of the high-burnup structure (HBS) in SCIANTIX, with the final goal of improving the description of pellet-cladding mechanical interaction. More precisely, the current model for HBS formation has been improved by a corroborated burn-up dependent uncertainty analysis and has been extended by accounting for a dedicated porosity in the HBS and their contribution to the local swelling strain. The analysis demonstrated that compared to state-of-the-art semi-empirical models, the newly proposed physics-based model presents slightly higher uncertainties, since it involves more parameters to describe the formation of HBS. Nonetheless, maximum uncertainty is observed at around 100 GWd/t, i.e., at the burn-up level at which the transition is almost completed, hence integrating the effect of all the involved parameters. A new numerical algorithm has demonstrated promising capabilities, targeting the description of the evolution of the HBS porosity. This capability is needed since (1) physics-based description of this phenomenon requires the solution of non-linear differential equations, for which numerical schemes available in SCIANTIX are not suited, and (2) the coupled description of the evolution of integral, mean and variance of the pore-size distribution requires high numerical accuracy and robustness since it is intended to inform fuel fragmentation models. Verification and Validation are ongoing, and the extended version of SCIANTIX should finally be coupled with TRANSURANUS. A code-to-code benchmark with MFPR-F is envisaged, too.

Other partners involved in this task have not started their work.

2.4 WP4-SGTR

2.4.1 Objectives

The main objectives of WP4 are to:

- Perform reviews of open literature (models and data) and experimental programmes for the fission product transport/behaviour in primary circuit and failed Steam Generator, for the gap release from defective fuel rods and iodine spiking phenomena and for the clad secondary hydriding in defective fuel rods in Normal operations
- Update/implement models in integral codes, fuel performance and clad behaviour codes
- Assess the revised/new models for DBA and DEC-A conditions against the tests included in the R2CA experimental database relevant for SGTR phenomena

The work-package is subdivided into 3 tasks respectively dedicated to:

- Task 4.1: Fission product transport and release from the primary circuit to the environment
- Task 4.2: Fission product release from defective fuel rod during SGTR transient (including the iodine spiking phenomena)
- Task 4.3: Secondary hydriding phenomena of defective fuel rods in normal operation and subsequent clad failure under SGTR transients

2.4.2 Overview of the main advances

The main progresses made during the second year of the project are briefly described below:

- Regarding the fission product transport/behaviour in the primary and secondary circuit (including the failed steam generator) an extensive effort was done by some partners to search for other available data beyond the R2CA database. These data are generally scarce but some were found in NPP reports. Reviews of the models included in some of the codes that will be used to simulate SGTR transients were initiated (RELAP-5, MELCOR, MAAP5). Needs for improvements were identified and in some cases already done as in MAAP5;
- Regarding the fission product release form defective fuel rods review of literature has also been performed and new data from NPPs identified. Some of these data were already used to improve the models as for instance the iodine spike modelling in RING code. Developments for fission releases in ANS5.4 and SCIANTIX are on-going and proposals for model enhancement in TRANSURANUS regarding the fission gases transport in hyper-stochiometric fuel made;
- Finally regarding the secondary clad hydriding, the bibliographic review of available models was finalized, new H_2 uptake experiments within 300-400°C were performed and model revisions/developments initiated (i.e. for radial redistribution and precipitation of H_2, diffusive mixing of gas in the fuel rod gap.

2.4.3 Details of the activities performed

2.4.3.1 Task 4.1: Fission product transport and releases from primary circuit to environment

The main objective of task 4.1 is to improve models and codes for the simulation of fission products behaviour during a SGTR transient with special attention to the FP transport and behaviour (especially for iodine) in the primary circuit and FP behaviour in failed steam generator release to the secondary side and environment. To do so, the database of fission product release and transport will be gathered and their suitability to the conditions of interest assessed. Proposals, if necessary, for improvement/adaptation of integral computer codes are foreseen.

The objective for this second year is to evaluate the progress of the assessment carried out by the partners, in compliance with the aforementioned objective. This information will be gathered in the planed deliverable "D4.1.1: Progress report on experimental database reassessment and on model/code improvements for fission product releases during a SGTR transient" at the end of October, 2021.

A brief information of the work done follows.

During the past year, EDF contribution to task 4.1 was dedicated to the analysis, enhancement and verification of the models implemented in MAAP for the FP releases from the primary side to the secondary side and eventually to the environment. Some improvements were made by considering specific of different FP species (noble gases, iodine, caesium…) and the potential overflow of the SG, which notably affects releases to environment.
Additionally, a new model was added in MAAP for iodine spiking during SGTR sequences.
The performance of the enhanced MAAP version was compared to COSAQUE (EDF reference code for activity calculations) predictions on 2 different types of plants: PWR900MWe (3 loops) and PWR1300MWe (4 loops). The enhanced MAAP resulted in estimates noticeable similar to COSAQUE ones. Such comparisons will be extended for more SGTR transients for the N4-type plant. Eventually, the intention is to activate those models for crises situation analyses (real crises or training exercises).

In BOKU, the target of the work is to enhance the RELAP5 capability to simulate the fission product transport and behaviour during SGTR transients in the primary and secondary circuit.
At present, the decay chains of fission products within the code have been analysed, possible shortfalls have been identified and vias of enhancement are being explored.
As for iodine spiking, an extensive literature survey has been conducted to find out enough data to model it with RELAP5. Very few data publicly available have been found, most data having been taken more than 3 decades ago. Some additional data have been found in individual investigations and nuclear power plants reports. The data gathered are mostly referred to Western PWRs and much fewer to Russian VVERs. This information is being used to build an external function that feeds RELAP5 as a FP source.

CIEMAT has started the review of the experimental data referred to in Task 2.1.3 of the R2CA project concerning the FP transport; a preliminary screening out of some of the data has been done. As a result, it has been concluded that few data are applicable to the transport processes that are postulated to dominate FP transport in the primary circuit and transfer to the secondary one during SGTR DBA and DEC-A sequences. A detailed evaluation of the database is being drafted and new sources of information are being reached beyond R2CA. At the same time, the implemented FP transport models in MELCOR have been examined and found to be applicable just in the secondary transport of FPs in the gas phase; the iodine models available in MELCOR are outdated and could not be applied under the secondary side conditions of a SGTR sequence.
A template for D 4.1.1 to gather all the partners contribution have been elaborated and released.

Other partners have not started their work. IRSN contribution on a fast evaluation of FP releases in the SAFARI code is planned from Jan. to May 2022. SSTC contribution on iodine spike effect simulation under SGTR accidents is planned August, 2022. UJV work was also postponed. It should be initiated before the end of this year. The literature and experimental program review should be completed by the end of this year and the ATHLET-CD model improvements will be finished during the first quarter of 2022.

2.4.3.2 Task 4.2: Fission Product release from defective fuel rods during SGTR

The main objectives of Task 4.2 are to better predict the complex fuel pellet behaviour of defective rods during a SGTR transient and the iodine spiking phenomena. It concerns:

- Fission product releases, especially iodine from defective fuel rods during SGTR transient
- Complex fuel behaviour in defective fuel rods (especially oxidation vs secondary hydriding).

Before detailing the recent progress obtained in this task, it is worth to summarize the status of the activities ongoing. The quantification of the impact on the rod failure on the fuel temperatures and hence microstructural changes and fission product release is ongoing (performed by UJV with TRANSURANUS simulation of VVER-1000 fuel rods – similar simulations are being prepared by SSTC-NRC). Also in progress is the implementation and further development of ANS5.4-2009 model in TRANSURANUS (ongoing by JRC) and in SCIANTIX (POLIMI), including the development of a methodology to bound the numerical error on the prediction of fission product released (work done in SCIANTIX, detailed in the following). Testing has been performed on the CONTACT1 experiment of the IFPE database (disseminated in two conferences and a submitted journal paper). Collaboration between IRSN and JRC demonstrated the proper functioning of the coupling of MFPR-F and TRANSURANUS that will be further used to evaluate the iodine release from defective fuel rods under SGTR conditions. BOKU started a PhD position focused on modelling of iodine spiking. Review of present literature is ongoing and modelling with RELAP5-3D is targeted. Improvement of iodine spiking modelling in the RING code is ongoing by EK (detailed in the following), via the evaluation of new NPP measurements. Modelling of fission product release from defective fuel is under development, additional models are/will be introduced in TRANSURANUS by NINE (detailed in the following). Review and evaluation of the experimental data, concerning FP release (based on the classification of the document D2.3 “Report on SGTR and LOCA available experimental data” and on available open literature), have been performed by CIEMAT. Review of the available MELCOR release model and determination of the potential improvement is ongoing.

In more details, CIEMAT plans to review the experimental data base on fission product release and to check the applicability of models currently existing in MELCOR 2.2 (CORSOR and CORSOR-Booth type). These tasks have been hardly started; a preliminary model assessment indicates that a potential application of the in-MELCOR models to DBA and DEC-A conditions during SGTR sequences is unlikely. If this preliminary observation is confirmed, an external function will be built to model iodine spiking.
Towards the improved modelling of iodine spiking, EK further developed the RING code against new 18 nuclear power plants measured datasets (during power transients, reactor shutdown and start-up). The targeted developments have been oriented to overcome the underestimation of the effect of the power change in previous version of the code, and the introduction of new cesium spiking models (^{134}Cs and ^{137}Cs). The upgraded RING code will be applied to the simulation of iodine and cesium spiking effect in SGTR, and collector cover opening conditions. In addition, it will allow 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. The original datasets used for the simulation of steady state and transient conditions with the RING code derived from the coolant analysis of the VVER Paks NPP, performed by the Institute of Nuclear Techniques of the Budapest University of Technology and Economics (BME NTI). The improved acceleration factor for the release has been tailored and tested against these data, resulting in more reliable predictive capabilities of the code itself.

NINE is currently carrying out the activity of implementation of analytical models for the prediction of FGR from defective fuel rods in the TRANSURANUS code. The first efforts of this activity went to the open literature research.

More than 20 papers and technical reports were analysed and finally three of them (Lewis (2017), Massih (2018) & Veshchunov (2019)) were taken as main reference for the TRANSURANUS models implementation:
The objective of the work is to implement the analytical models and correlations described in the reference literature in the TRANSURANUS code, which has been done through the extension of existing Fortran 95 subroutines and the definition of new subroutines following a graded approach.
The FGR in defective fuel rods is split into 2 steps: the release from the fuel matrix to the fuel-cladding gap and the subsequent release from the gap to the coolant through the defect opening. The fission gases diffusion inside the fuel matrix is already implemented in TRANSURANUS and different models are available. Starting from the existing model of the extended mechanistic model by Speight, some improvements are introduced. In particular, the deviation from the stoichiometric fuel condition is considered. The UO_{2+x} fuel matrix results in a greater mobility of the fission products and as a consequence an enhanced release behaviour from hyper-stoichiometric fuel. This important effect is described by the correlation of Kim from Massih (2018*)* that has been implemented in a new subroutine. This model can be selected directly from the input file as a new option. Furthermore, some verification code runs have been performed to compare the FGR starting from the same rod conditions and selecting the new or the original diffusion model. The effect of the enhanced diffusion was confirmed from these demonstrative simulations.
The next step will regard the modelling of the FGR from the gap to the coolant. This capability is not implemented in the TRANSURANUS code, since it does not consider defective fuel rods. The reference paper by *Veshchunov* describes different release models depending on the half-lives of the isotopes. At the current state of the code, the isotopes are not separated and just a single value obtained summing the Xenon and the Krypton contribution to the FGR is provided in the simulation output files. For this reason the source code will be modified in the following way:

- Separate the contributions from the different fission products isotopes to the FGR, for both stable and unstable species.
- Adopt the suitable FGR model depending on each isotope half-life as described by Veshchunov.
- Enlarge both the FP species and the isotopes considered in TRANSURANUS, most important introducing the (most relevant) Iodine isotopes.

The implementation of the above listed capabilities requires to introduce a large number of modifications in the existing subroutines and also to define new subroutines to predict the release to the coolant for defective fuel rods. The complete development of the FGR from defective fuel model is planned to be concluded by mid November 2021 so to have time to perform the verification and validation activities and eventually modify correlations subroutines based on V&V feedback. The V&V will be performed by comparing the TRANSURANUS simulation results with a reference defective fuel rod experiment that was conducted for investigating model response under SGTR conditions. The final extended feature of the TRANSURANUS code is planned to be ready by December 2021. The development of the FGR from defective fuel is conducted under a bilateral agreement signed with JRC, which is the TRANSURANUS code developer.

Complementary with the modelling effort by NINE, POLIMI developed an a priori methodology to bound the numerical error on the prediction of fission product/gases release. The proposed methodology, tailored to state-of-the-art spectral diffusion algorithms, takes off from a parametric error analysis, involving the number of time-steps and the number of modes used in the computation of the numerical solution. Exploiting the triangular inequality, an upper bound of the error is defined, as a function of the number of time-steps, the number modes, and specific irradiation conditions. The outcome of the error analysis is a set of reference tables collecting fitting factors for the error bounds. The operative procedure to bound the error in constant conditions is thus: (1) fix the demanded error upper bound (e.g., 0.5%), (2) estimate the non-dimensional characteristics of the irradiation history and choose the number of time-steps and the number of modes for which the fit function provides a value below the demanded upper bound. The described procedure is applicable both in constant and in transient conditions and is thus viable for application in the cases of interest for the project.

SSTC NRS has started already the open literature search with respect of investigation of fission product release from fuel pins under primary to secondary leaks. Main attention was paid on investigation approaches for iodine spike-effect modeling. With this respect we analyzed the following sources:

- Kurchatov Institute document “Calculations of the fission products inventory under the cladding of hermetic and unhermetic fuel elements of VVER-1000 fuel assemblies (TVSA, TVS-2) with deep fuel burnup (60 MW * day / kg uranium for the fuel element) and the activity of the primary coolant. Report of the RRC KI, M: - 2004
- Issue 197 "Iodine spiking phenomena" of document “NUREG-0933. Resolution of Generic Safety Issues (Formerly entitled "A Prioritization of Generic Safety Issues"), Main Report with Supplements 1–34, 2011
- Regulatory Guide 1.183 “ALTERNATIVE RADIOLOGICAL SOURCE TERMS FOR EVALUATING DESIGN BASIS ACCIDENTS AT NUCLEAR POWER REACTORS”.

As an option we are considering to collect data for iodine spike-effect issues for Ukrainian NPPs.
The work is still being performed (we had some delays for performing). The preliminary data for finalization April 2022.

References

B.J. Lewis, P.K. Chan, A. El-Jaby, F.C. Iglesias, A. Fitchett, (2017), “Fission product release modelling for application of fuel-failure monitoring and detection - An overview”, Journal of Nuclear Materials, 489, pp 64-83.
A.R. Massih, UO_2 fuel oxidation and fission gas release, (2018), Report number: 2018:25, Swedish Radiation Safety Authority/Stral Säkerhets Myndigheten, Quantum Technologies AB.
M.S. Veshchunov, 2019, “Mechanisms of fission gas release from defective fuel rods to water coolant during steady-state operation of nuclear power reactors”, Nuclear Engineering and Design, 343, pp 57–62.

2.4.3.3 Task 4.3: Secondary hydriding phenomena

Main objectives of this task during the three years of its duration are:

- To investigate the secondary hydride formation on the inner part of the clad of a defective fuel rod during normal operation and SGTR transients and develop suitable models;
- To evaluate the impact of secondary hydriding on subsequent fuel rod failure through clad mechanical embrittlement
- To determine a failure criterion for defective fuel rods (ductile-to-brittle transition criterion)

After the performance of bibliographic review of available models in open literature and assessment of the capabilities of the models in the codes to be used within the project, the objective of the 2nd year was mainly:

- to develop or adapt existing models for H_2 uptake, H_2 migration/radial distribution and hydride precipitation as well as models for gas diffusion in the fuel/clad gap
- To implement these new/revised models in the codes to be used for SGTR reactor calculations (i.e. FRAPCON, SHOWBIZ, TRASURANUS...)

The understanding and detailed numerical modelling of the physical mechanisms involved in the secondary hydriding phenomena need experimental data, which are representative for the physical parameters of the nuclear power plants (NPP). For the gaseous hydrogen uptake of Zr, a large number of tests are available, but most of them were carried out at high temperatures. In the defective fuel rods, during normal operational conditions, the typical cladding temperatures are in the range of 300-400 °C.

MTA-EK successfully completed experimental series with hydrogen charging of Zircaloy-4 and E110 alloys in the laboratories of Centre for Energy Research (MTA-EK).

- The tests covered the temperature range of 300-400 °C.
- The experimental data showed the increase of hydrogen uptake with the increase of temperature.
- The hydrogen uptake of the two tested alloys was significantly different.

The technical report EK-2021-437-1-1-M0 describes the experimental program. The experimental data were collected, and the database is available for model development purposes. The detailed information included in the database will allow the R2CA participants to improve numerical models on the H uptake process.

IRSN completed a review of available literature on secondary hydriding phenomena and of French Nuclear Power Plants experience of defective fuel rods during normal operation. Since the first observations of such degradations, especially for boiling water reactors, scenarios have been proposed to explain the origin of secondary hydriding. Among the mechanisms involved, some of them are now widely accepted and have been confirmed by a few integral tests. This is the case of the internal oxidation of the cladding as a source of hydrogen or steam depletion conditions necessary for massive hydriding. However, the kinetics and triggering of such hydriding are still subject to controversy. For instance, incubation times, internal communication of gaseous species and loss of protection by the internal zirconia are still open questions.

This bibliographic report has made it possible to establish a scenario for an implementation in SHOWBIZ code. This scenario was built from SHOWBIZ version V1. It takes advantage of laws already implemented in SHOWBIZ and which will be parameterised based on experimental results found in the literature, in particular the clad oxidation and hydration rates. The implementation of a model inspired by the Veschunov's model have been established to treat the gas mixture/transport in the gap. A massive hydriding model compatible with the SHOWBIZ software architecture is envisaged.
IRSN has developed and tested the dedicated CHANNEL module in SHOWBIZ software where the internal gas mixture and transport is calculated together with the interaction with the inner side of the fuel rod clad. Coupling with the chemical models have also been developed and successfully tested. The first demonstration calculation have been done for numerical verification and already shows the great relevance of internal oxidation kinetics.

The CIEMAT´s technical program so far has dealt with the modelling of the in-clad secondary hydriding process. To do so, the following tasks have been carried out:

- Adaptation of previous CIEMAT's attempts to model hydrogen migration/precipitation throughout the cladding. Particularly, the CIEMAT´s model has been adapted to cladding fuel side hydrogen uptake and with alternative options in the precipitation modelling, both adapting a new model (more phenomenological) and accounting for a wider variety of solubility limits found in the literature.
- Adaptation of FRAPCON-4.0 to corrosion and hydrogen pick up in the cladding fuel side.
- Coupling of CIEMAT´s model with FRAPCON-4.0.

The modelling has been assessed against postulated scenarios of massive hydrogen pickup in the cladding fuel side at the beginning of life. The results obtained point out that the predictability enhancement of the in-clad hydrides distribution implies to properly model the hydrogen precipitation with a more phenomenological approach. In this regard, further verification/validation is foreseen based on data made available. To do so, further adaptation is foreseen to be done in order to properly simulate the boundary conditions anticipated in defective fuel rods.

As mentioned in the previous report, the JRC has implemented and tested the new model for hydrogen uptake under transient conditions in collaboration with NucleoCon, which complements the previous work in the frame of the ESSANUF project (Gyori et al (2017)).
Also JRC started the development of a model for radial redistribution of hydrogen in zircaloy cladding. As outlined in the previous yearly report, it was initially decided to consider harmonisation of the other radial distribution models of TRANSURANUS such as OXIRED (Lassmann (1987)), PUREDI and AMREDI (Di Marcello et al (2014)).
In fact two models are currently under development. The first model relies on the numerical technique applied in the PUREDI model (Di Marcello et al (2012)), whereas the second model is developed in collaboration with K. Lassmann and relies on the same numerical technique as the revised OXIRED model.
Both models have been tested in a separate environment, which led to select the second model for implementation in the latest version of the TRANSURANUS code prior to distribution to the user network. The revision of OXIRED not only considers the upgrading of the correlation for the heat of transport and corrected the balance equation for the average oxygen concentration by considering the un-deformed pellet radius, it mainly involves a new transient solution that complements the previous approximation of OXIRED. It relies on the finite difference formulae for unequal intervals based on Lagrange's interpolation with an implicit time integration. Careful testing and

comparison with the work of Forsberg et al (2020) and the previous OXIRED model has been completed in a separate environment, and it has been implemented in the latest version of the TRANSURANUS code (V1m5j21). This implementation requires some additional changes (e.g. unit adaptation, variable renaming, etc…) which are currently under way and requires the development and testing of a separate time step control mechanism for the hydrogen redistribution model.
As the coupling of MFPR-F and TRANSURANUS codes has been successfully demonstrated for LOCA conditions (see in task 3.3.), the simulation of the effect of stoichiometry variations can also be envisaged. It requires the implementation of a time-varying boundary condition in the new version of OXIRED, and an additional model for predicting the variation of the oxygen partial pressure in the gap that will provide the boundary condition for OXIRED in each axial slice.

Other partners involved in this task have not started their work.

References

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V. Di Marcello, A. Schubert, J. van de Laar, P. Van Uffelen, 2012, “Extension of the TRANSURANUS plutonium redistribution model for fast reactor performance analysis”, Nuclear Engineering and Design, 248, pp 149.
M.S. Veshchunov, 2019, “Mechanisms of fission gas release from defective fuel rods to water coolant during steady-state operation of nuclear power reactors”, Nuclear Engineering and Design, 343, pp 57–62.

2.5 WP5-INNOV

2.5.1 Objectives

The main objectives of WP5 dedicated to innovation are to:

- Identify then evaluate with the improved calculation scheme developed within the project the gains of potential new accident management actions/procedures and devices (including specific instrumentation) but also of some concepts of Accident Tolerant Fuels;
- Explore the capabilities of diagnosis/prognosis evaluation tools based on AI to anticipate an on-going accidental situation especially for the cases with defective fuel rods.

The work-package is subdivided into 3 tasks respectively dedicated to:

- Task 5.1: The identification and evaluation of pro & cons of innovative devices and management approaches
- Task 5.2: The development of innovative diagnosis tools
- Task 5.3: To the evaluation of Accident Tolerant fuels focussing in a first intention on the most promising and mature ones.

2.5.2 Overview of the main advances

The main progresses made during the second year of the project are briefly described below:

- In task 5.1, the identification of innovative devices and management approaches based on open literature survey and from Test-Facilities to reduce the consequences of some scenarios is also almost completed. A questionnaire on actual status and main requirements for the new devices/procedures was also elaborated. Distinctive features at the initial stage of PRISE leakage accidents in VVERs-1000 as well as timing for decision-making and for taking management measures were analysed. Based on this analysis, some automatic algorithms were developed and are currently under assessment and evaluation regarding their effect on Radiological Consequences;
- Regarding innovative diagnosis tools a literature review on “Artificial Intelligence” (AI) application in non-nuclear fields was performed for ruling on its potential application in managing NPP safety. The preliminary result of the performed analysis provided by NINE, currently suggests focusing on the term of “expert system” instead of “artificial intelligence”. Expert system is a system capable to execute a list of instructions for a given input, but it is also capable to redefine its goals not included in its original programming on the base of the occurring conditions. In parallel, preliminary specifications have been developed for a simplified tool based on AI to be used to anticipate the on-going situation in a plant with defective fuel rods;
- Finally regarding the work on Accident Tolerant Fuel a bibliographic survey focused on the short-term concept of Chromium coated Zr-based materials was performed to identify the relevant parameters (i.e. physical, chemical and mechanical properties) to be considered in the calculations. In parallel experiences gained form the IL Trovatore EC project on other ATC concepts are currently collected that will be used to feed the review. Some extension of the fuel performance codes with various materials properties and models have already been performed (i.e. in TRANSURANUS) as well as specific code improvements necessary to perform the uncertainty/sensitivity study on ATFs.

2.5.3 Details of the activities performed

2.5.3.1 Task 5.1: Innovative devices and management approaches

About the identification of innovative devices and approaches, it is necessary to evidence that the development of new devices and approaches in the management of the NPP during accident occurrence is a process that typically requires a large effort to demonstrate its effectiveness and applicability. As a consequence, in this task, it cannot be proposed innovations that are generally developed by large companies with large resources. However a strategy has been proposed to perform this subtask. This strategy is based on the identification of the devices and procedures adopted in the experimental facilities and to consider their possible implementation in the NPP. In the NPP the priority is typically given to the management of the plant for normal operations. Concerning the control of accidents progression and the actuation of the safety systems, a reduced set of signals are necessary and implemented. This approach, of course, also is due to a conservative approach that does not require a fine representation of the plant conditions in accident situation (e.g. only the temperature the core outlet temperature is conservatively necessary for emergency response, and the details of the outlet temperature at different core zones (or channel) is not requested). However, this approach strongly limits to derive details on the plant status and to develop less conservative and more punctual responses to accident occurrence. On the opposite in the test facilities basically all the instrumentation is devoted to the monitoring the accident progression details. The idea is to transport some of these experimental facility solutions in the NPP for application to derive new approaches.
The possible applicability and advantage of test facilities instrumentation and procedures are collected and evaluated for possible application in NPPs and for potential advantages in managing their accidental conditions.

Concerning this aspect, a technical note has been prepared (currently in draft version to be finalized) jointly by NINE and BOKU including the description of the currently adopted procedure and devices in the NPP (BOKU) and the identification of the possible test facilities devices and procedures useful for NPP accident management procedures.

A questionnaire has been set up by NINE in to be circulated among the partner, to have a global view concerning the meaning of innovative devices and procedures, what is considered as desirable to develop, for what kind of NPP their application is useful and if the development of innovative devices and procedures is a process they perform(ed) and the dedicated resources.

At the current stage of Task 5.1 ARB's efforts are focused on AM strategy for PRISE leak accident.
To date, within the framework of the AM strategy, the following was completed:

- Preliminary calculations were carried out to study the distinctive features at the initial stage of the accident and the timing for decision-making, as well as for taking management measures.
- Based on the results of the work, a preliminary concept of the accident management strategy in the event of a PRISE leakage accident at VVRs-1000 was developed.
- All accident management actions in accordance with the adopted strategy, as well as in accordance with the procedures prescribed in the plant emergency instructions, were organized as a set of sequential actions that must be sequentially implemented within a certain (sufficiently short) period of time. The complete list of actions is divided into separate groups in the form of separate logical controls and is presented in the form of a logical diagram with actions that are performed on a time basis (one-time actions) or on a symptomatic basis (monitoring actions).

Further ARB's steps will focus on:

- Analysis of the automatic Algorithm architecture. Development of automatic algorithms for SGTR management for VVER-1000.
- Analysis of the Preconditions for starting of accident control.
- Assessment of Applicability of the Algorithm for PRISE leak range of 10÷100 mm leaks.
- Operation of the Algorithm under DBA and DEC-A conditions. An assessment of the effect of the algorithm on RC (comparison of RC without and with the algorithm).

2.5.3.2 Task 5.2: Innovative diagnosis tools

The activity performed by NINE was focused on the possible application of artificial intelligence in managing safety of the NPPs. At lowest levels intelligent systems are identified with systems efficiently and in a short time capable to extract patterns hidden in large data base. In this case the system can suggest some "structure" from the raw data, to derive a more appropriate response for different situations. It can be an applicable approach in the NPP accident management procedure, but a large amount of data is necessary.
However the most advanced intelligent systems are not limited to the data analysis, but are developed to take decision also in situations when not all the necessary data are available. This is a complex approach because many aspects are connected. As an example, use of artificial intelligence posed a lot of relevant aspects: what are the signals to consider, how to read the signals, how to interpret and how to manage the signals.
It is also a complicated approach because the definition of artificial intelligence is currently different for different applications.
The preliminary result of the performed analysis currently suggests focusing on the term of "expert system" instead of "artificial intelligence". Expert system is a system capable to execute a list of instructions for a given input, but it is also capable to redefine its goals not included in its original programming on the base of the occurring conditions. Of course, the validation of such an approach require to define new procedures and standards.

The work planned by IRSN within the framework of this task relates to the development of advanced tools to better anticipate the on-going situation during a transient (SGTR and LOCA) and to help the accident management.
The first works performed concern the specifications for the simplified AI tools (leaking fuel rods) and the bibliography of AI tools.
A post-doctoral program including the development and validation of the simplified tool, then the database generation, will start soon (the candidate has been selected). The physical model, in order to satisfy the need for a fast tool linked to the production of several million calculations, will be a meta-model resulting from simulations using the MFPR-F code, under development at IRSN. In a first step, the adaptation of the MFPR-F code to the problem to be addressed will require the development of a model for the recoil and ejection of fission products in the free volume of the fuel.
In a second phase, new models will be developed to deal with the following phenomena:

- The behaviour of iodine, in terms of release from the fuel and possible retention in the free volume ;
- The release of fission products from the gap into the primary circuit; Veschunov's model might be used for this purpose ;
- Radioactive decay in the free volume. The ISODOP module available in the ASTEC code might be used as a basis.

These models will be "chained" with the MFPR-F code in order to have a tool covering all the phenomena. By this way, we will carry out the calculations for building the meta-model. Once generated database, IRSN will develop and validate the diagnosis tool by using a machine-leaning algorithm.

References

M.S. Veshchunov, (2019), "Mechanisms of fission gas release from defective fuel rods to water coolant during steady-state operation of nuclear power reactors", Nuclear Engineering and Design, 343, pp 57–62.

2.5.3.3 Task 5.3: Advanced Technological Fuels

The main objective for the second year was to identify the relevant parameters and needed laws/material properties for the Accident Tolerant Fuels and to review the different code capabilities that will be used to perform the uncertainty/sensitivity analysis (DRACCAR, FRAPCON/FRAPTRAN, TRANSURANUS).

EDF has performed an exhaustive bibliographic review concerning thermo-physical, mechanical behavior and oxidation kinetics on Zr coated Cr cladding and Cr doped and high density fuels. Secondly, thanks to the bibliographic review EDF has proposed new models for oxidation kinetics and creep laws for Zr coated Cr cladding.

The JRC contributed to the literature review on other ATF concepts based on experiences gained in the frame of the Il Trovatore project and work done in the frame of International organisations that are listed in Table 2 and Table 3.

Table 2: List of project activities related to eATF organised by the IAEA

Project Acronym	Time frame	Scope	Reference
ACTOF			
ATF-TS	2020-2023	Single rod and bundle tests on ATF performance under normal, DBA and DEC conditions Code benchmarking Development of LOCA evaluation methodology for ATF	https://nucleus.iaea.org/sites/connect/NFEpublic/Pages/ATF-TS.aspx In progress

Table 3: List of project activities related to eATF organised by the OECD-NEA

Project Acronym	Time frame	Scope	Reference
EGATFL	2014-2018	State-of-the-art report	NEA No 7317, 2018 (https://oe.cd/2mL) https://www.oecd-nea.org/science/egatfl/
TOPATF	2018-2020	Technical Opinion Paper on Safety Criteria for Accident-Tolerant Fuels	Publication in progress
HRP	2015-2020	In-pile experiments with single rods with doped fuel and/or different ATF cladding materials	https://ife.no/en/tag/halden-reactor-project/ (HWR-1274)
SCIP IV	2019-2024	Out-of-pile fuel fragmentation tests (LOCA conditions) with additive fuels as ATF materials	https://www.studsvik.com/scip-project/scip-iv/
INCA (proposal)	2021-2024	Compare in-pile creep of ATF cladding materials (coated Zry) with conventional Zry for VVER-1000 reactors.	https://www.oecd-nea.org/download/science/workshops/neaframework/
QUENCH-ATF (proposal)	2021-2024	Integral out-of-pile LOCA bundle test to compare FeCrAl and optZIRLO. Complement to previous QUENCH19 test.	https://quench.forschung.kit.edu/ https://publikationen.bibliothek.kit.edu/1000089029

In addition, the JRC extended the TRANSURANUS code by implementation of materials properties for FeCrAl cladding in collaboration with NINE. In addition, the statistical post-processing program TUPython of the TRANSURANUS package was further improved in order to support the Best Estimate Plus Uncertainty (BEPU) analyses. Thanks to the Monte Carlo input sampling approach, uncertainties of up to 40 safety-relevant modelling variables can be statistically estimated. In a paper submitted to TOPFUEL2021 conference to be held in Santander, Spain from 24-27 October 2021, the main functionalities of this tool were outlined and illustrated using a test case and a numerical experiment based on Wilks' formula. More precisely, we illustrated how the standard statistics can be calculated with the new graphical user interface and demonstrated a numerical experiment with 1st to 6th order Wilks' methods. Based on the numerical experiment we showed that the 1st order Wilks' method for calculating the 0.95/95% uncertainty estimator contains also uncertainty in itself and can deliver very conservative values for a safety-relevant variable. This work has been submitted in a paper submitted to TOPFUEL2021 conference to be held in Santander, Spain from 24-27 October 2021.

Finally, in JRC, the statistical post-processing program TUPython of the TRANSURANUS package was further improved in order to support the Best Estimate Plus Uncertainty (BEPU) analyses. Thanks to the Monte Carlo input sampling approach, uncertainties of up to 40 safety-relevant modelling variables can be statistically estimated. In a paper submitted to TOPFUEL2021 conference to be held in Santander, Spain from 24-27 October 2021, the main functionalities of this tool were outlined and illustrated using a test case and a numerical experiment based on Wilks' formula. More precisely, we illustrated how the standard statistics can be calculated with the new graphical user interface and demonstrated a numerical experiment with 1st to 6th order Wilks' methods. Based on the numerical experiment we showed that the 1st order Wilks' method for calculating the 0.95/95% uncertainty estimator contains also uncertainty in itself and can deliver very conservative values for a safety-relevant variable.

Tractebel has reviewed the applicability of the key models in FRAPCON/FRAPTRAN for simulation of the ATF behaviour of coated cladding during Loss-Of-Coolant Accident (LOCA). Some scoping studies have been performed to test of feasibility of using the current version with specific model options to simulate the impact of coated cladding. It was concluded that additional model development is needed, such as the specific models for steady-state corrosion, high temperature oxidation and creep, as well as the burst criteria. These developments will be carried out particularly within the R2CA project.
IRSN has not yet started the work. It is planned to be done in 2022 after the work regarding the ATF needed laws will be finalized.

2.6 WP6-DISSE

2.6.1 Objectives

Informing society about the project and its results, going beyond the project's own community, is one of the key elements of H2020 projects. The communication, together with the dissemination and exploitation, is necessary to demonstrate and maximize the societal and economic impact of Project and shows the impact and benefit of European Research and Innovation funding. The main target of the communication activity is to communicate and promote the project by informing about the project itself and its results. The main target of the dissemination activity is to describe and make results available for use. The main target of the exploitation activity is to make use of the project results.
The objectives of WP6 for the second year of activity were to:

- Disseminate the ongoing project results;
- Perform the training on SCIANTIX agreed at the 1st annual meeting;
- Post the project updates and deliverables on the social channels;
- Issue the 2nd newsletter;
- Complete the website;
- Continue to follow the mobility program.

Due to the COVID19 pandemic, the workshop planned at the end of the second year of the activity was postponed. Its organization will be discussed in the third year of the activity. In the organization of the workshop, potential interested organizations will be contacted to invite them to participate to the End User Group.

2.6.2 Overview of the main advances

Considering the previous objectives, the following activities have been done along the second year of activity:

- 11 presentations in conference: 9 in 2021 (NENE, SNE, TOPFUEL, TU int WS) + 2 in 2022 (NURETH19, ERMSAR22);
- 2 journal papers: Nuclear Engineering and Technology by POLIMI;
- 1 generic presentation of the project by video planned for NURETH19;
- 2nd newsletter issued;
- All public deliverables archived in Zenodo (R2CA project community) and shared through social networks and R2CA public website;
- Mobility (6) not yet started;
- PhD (1) / MScs (2) in progress in BOKU/POLIMI, post doc to be started in September in IRSN;
- 1 online SCIANTIX training performed on October 16th, 2020;
- Posts on Linkedin and ResearchGate;
- R2CA website is online (https://r2ca-h2020.eu/);

Overview of the main advances towards the specified objectives including, when appropriate, a summary of deliverables and/or milestones, and a summary of main results.

In relation to the WP6 deliverables (D6.1 and D6.2), they have been released during the first year of the project.
In relation to the WP6 milestones, the MS9 and MS10 (due date: month 44) are not part of this reporting period.

2.6.3 Details of the activities performed

2.6.3.1 Task 6.1: Education and Training

In relation to the education and training task, education and training needs have been collected through the Partners and an updated list of mobility, Table 4, master thesis, Table 5, and training session proposals, Table 6**Erreur ! Source du renvoi introuvable.**, are available.

After R2CA 1st Yearly Progress Meeting, an online training course about the SCIANTIX code has been performed on October 16, 2020. 30+ participants from both institutions within and outside the consortium of R2CA joined the course. 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 material used in the Training (slides, case studies with related documentation) is publicly available, together with the source code of the SCIANTIX version used. The recording of the Training is also available, divided in six videos covering all the topics presented.

Table 4: Mobility proposal collected

#	WP / Task	Duration	Staff involved (MSc student, PhD student, Post-doc)	Envisaged period	Home organization	Host organization	Supervisor home organization	Supervisor host organization	Contact	Scientific objective	Justification for mobility
1	4.2	3 months	Post-doc	To be defined	POLIMI	JRC-Ka	Lelio Luzzi	Paul Van Uffelen	lelio.luzzi@polimi.it ; paul.van-uffelen@ec.europa.eu	1) Finalize the interface between SCIANTIX and TRANSURANUS and adapt code for inclusion of the new ANS5.4 model in the code 2) Model benchmarking (with MFPR-F, ANS5.4, FISPRO2)	1) Direct interaction with TRANSURANUS developers allows for speed up in identification of needs and problem solving 2) additional experimental data available at JRC can be used for code validation
2	4.3	1 month	PhD/Post-doc	To be defined (2022)	POLIMI	CIEMAT	Lelio Luzzi	Luis E Herranz	lelio.luzzi@polimi.it ; luisen.herranz@ciemat.es	Couple SCIANTIX with FRAPCON/FRAPTRAN in order for the fuel performance code to benefit from the envisaged work on fission gas behaviour modelling	Direct interaction with the users of FRAPCON/FRAPTRAN allows for speed up in identification of needs and problem solving
3	2.6	1 to 3 months	MSc student	To be defined (internal check on feasibility is on going)	POLIMI	Bel V	Lelio Luzzi	Albert Malkhasyan	lelio.luzzi@polimi.it ; albert.malkhasyan@belv.be	Fuel behaviour calculations with TRANSURANUS/ SCIANTIX of Belgian PWR-1000 fuel to complement CATHARE and MELCOR calculations performed by Bel V	Evaluation of interest and feasibility of proposal of new simulation strategies and best practices proposals for safety assessments
4	3.2	2 months	PhD student	To be defined (2021)	LEI	IRSN	Tadas Kaliatka	Francois Kremer	tadas.kaliatka@lei.lt; francois.kremer@irsn.fr	Evaluation of thermo-mechanical and thermo-chemical property evolution of BWR fuel by means of MFPR-F, which will be coupled with TRANSURANUS	Direct interaction with the developers of the MFPR-F code allows for speed up in identification of needs and problem solving, especially when coupling with the TRANSURANUS code (under development at IRSN and JRC)
5	4.2	1 - 2 months	PhD/Post-doc	To be defined	BOKU	NINE	Nikolaus Müllner	Marco Cherubini	nikolaus.muellner@boku.ac.at	Reevaluation of the fission product transport SGTR transient	Direct access to expertise. Feedback and improvement of the developed models.
6	5.1	1 - 2 months	PhD/Post-doc	To be defined	BOKU	NINE	Nikolaus Müllner	Marco Cherubini	nikolaus.muellner@boku.ac.at	Optimisation of accident management, evaluation of measures and benefits.	Direct Interaction with the task leader, feedback on and discussion of AM measures

Table 5: Thesis proposal collected

#	WP / Task	Duration	Envisaged period	Supervisor	Contact	University	Scientific objective	Candidate
1	4.2	9 months (MSc)	Nov 2020 - July 2021	Lelio Luzzi	lelio.luzzi@polimi.it	POLIMI	Include a new model for radioacive fission product release (new ANS5.4) in the SCIANTIX code. Improvements to the model are going to be considered along the thesis work, along with benchmarking	Giovanni Zullo
2	5.2	24 months (post-doc)	2021-2022	Karine Chevalier-Jabet	karine.chevalier-jabet@irsn.fr	not yet known	Quantify uncertainties related to the FP behavior in fuel/primary circuit. Build and validate a fast physical model for the behaviour of contamination in fuel/primary circuit aggregating the results of detailed codes and their uncertainties	
3	2.3/2.5/4.1/4.2/5.1	36 months(PhD)	2020-2023	Wolfgang Liebert/Nikolaus Müllner	nikolaus.muellner@boku.ac.at	BOKU	Investigation of Iodine Spiking phenomena, thermal hydraulic modelling of SGTR DBA and DEC-A scenarios, evaluation of accident management measurements to reduce the transport of Iodine to the secondary side and the environment.	Raphael Zimmerl
4	2.3/2.5/4.1	12 months (MSc)	2020-2021	Wolfgang Liebert/Nikolaus Müllner	nikolaus.muellner@boku.ac.at	BOKU	Validation of nodalisation-approach against PSB test facility experiments for a SGTR scenario. Utilization of our validated nodalisation in analyzing a steam generator tube rupture in a VVER 1000/320 reactor including source term evaluation	Lukas Anzengruber
5	3.3/4.3	9 months (MSc)	Mar 2021 – Dec 2021	Lelio Luzzi	Lelio.luzzi@polimi.it	POLIMI	Improve the modelling of HBS in SCIANTIX by the implementation of a dedicated numerical scheme	Bertin Meleqi

Table 6: Training proposal collected

#	Code / subject	Duration	Envisaged period	Host organization	Lecturer/Tutor	Proprietary issues for training purpose (Yes/No)	Contact	Other Notes
1	TRANSURANUS / fuel performance code	1 week	June 2021 ??	JRC-Ka	P. Van Uffelen, A. Schubert, Z. Soti (JRC)	yes, organisation sending trainee must have a TRANSUNANUS user licence agreement	paul.van-uffelen@ec.europa.eu	laptops of JRC are made available for trainees during course
2	SCIANTIX / meso-scale code for fission gas behavior modelling	1 day or two half days	R2CA 1st progress meeting (On-line, October 16, 2020)	ENEA-POLIMI	D. Pizzocri and/or L. Luzzi (POLIMI)	No (SCIANTIX is open source software)	lelio.luzzi@polimi.it	Traning sessions can be organized / carried out using participants' laptops
3	DRACCAR/ 3D Thermo mechanical code	3 days	2022	IRSN	S. Belon/T. Glantz (IRSN)	yes, organisation sending trainee must have a DRACCAR user licence agreement	gaetan.guillard@irsn.fr	IRSN laptops or participant laptops if trainees have a DRACCAR user license agreement

2.6.3.2 Task 6.3: Communication and Dissemination activities

Along this second reporting period, the following activities have been done:

- The second R2CA newsletter has been issued (front page in Figure 1);
- 10+ posts on Linkedin and ResearchGate;
- The public website, accessible at the following address https://www.r2ca-h2020.eu/, was developed. This HTML website is dedicated to the dissemination of the project information to the scientific community;
- Several scientific publications:
  - 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.
  - I. 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.
  - 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", Journal of Nuclear Engineering and Technology, 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.

R2CA Newsletter

Issue 2

28/08/2021

What's new in R2CA

The project is now in its second period. After the first year, the consortium members were brought together in a webinar to discuss the main achievements, the work plan for the future and identify potential issues. **Despite the health crisis, most of the work has been carried out on time.**

The first-period work was focused on reactor calculations of accidental scenarios and their associated release evaluations. The numerous results obtained should be presented outside the consortium next year at a dedicated open workshop.

Some of the project advances can be summarized as follows:

- **About 48 accidental scenarios** (both LOCA and SGTR) **were calculated on different kinds of reactor designs** (VVERs, PWRs, EPR and BWR), covering both DBA and DEC-A conditions, a simplified radiological evaluation tool was built ;
- **22 tests related to Zr-4 and E110 Hydrogen uptake in representative conditions of SGTR transients** (300-400°C) **were carried out** for clad hydration model upgrading ;
- **24 sets of reactor measurements of the iodine activity increase in primary circuit during power transients were provided** for iodine-spiking model improvement ;
- **1409 were selected from the collected burst test results**, for the future development of a new burst criterion based on clad stress ;
- **9 related publications were produced**.

In parallel, the R&D in support of the model improvement was initiated. First reports, to be published in August, should already contain interesting information concerning clad burst failure, secondary hydriding, fission product releases from defective rods, iodine partitioning in damaged steam generators, behavior of high BU fuel zone during transients.

Nathalie Girault, IRSN

SCIANTIX Course

On October 16, 2020, we held the first online SCIANTIX Training Course. 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 is being 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) **is publicly available, together with the source code of the SCIANTIX version used**. The recording of the Training is also available, divided in six videos covering all the topics presented. We take the occasion to thank all the participants to this first online training and look forward to organizing other activities!

L. Luzzi, POLIMI

Figure 1: Front page of the 2nd R2CA Newsletter

3 CONCLUSIONS

In this report were described the work status and the main progress accomplished by each of the consortium partner during the second year of the project covering the period September 2020-August 2021. This period, still marked by the health crisis, has made interactions more difficult and has forced us to organize all meetings at a distance. Even if it is still difficult to quantify the impact that this situation has had on the progress of the project, it is clear that this has not facilitated synergies and the pooling of tasks in a project where many actions were already independent and that this has strongly penalized the education and training actions (mobilities and training sessions on simulation tools postponed ...) and to a lesser extent those of dissemination (postponement of the open Workshop). It is remarkable to note, however, that despite these highly un-favourable conditions, an online training session on the SCIANTIX tool was nevertheless organized in fall 2021. It should also be noted that during this period no less than 10 papers have been produced related more or less directly to the project.
In spite of this, one of the major objectives of the coming year will therefore be to revitalize the common work (by promoting common publications, knowledge/data/model exchanges, mobilities between partner's organisation…) and to increase the visibility of the project outside (through the open workshop organisation, the End-User group set-up…).

One of the main advances of the project during this period was the finalization of all accidental scenario calculations covering LOCA and RTGV accidents under DBA and DEC-A conditions, the results of which were recorded in individual technical reports. About 48 scenarios were calculated on different kinds of reactor designs (VVERs, PWRs, EPR and BWR). A synthesis of these results is currently in progress and should make it possible to highlight the possible ways of improvement in the calculation chains to allow a better estimation of the radiological consequences of these accidental sequences. All the work that will allow to highlight the improvements made during the project and prepare the database has also been finalized (i.e. elaboration of simplified calculation tool for radiological consequence evaluation, excel data file for gathering the calculation results).

With regard to the work packages dedicated to R&D (i.e. WP3-LOCA & WP4-SGTR) and mainly to the improvements of the modelling of the phenomena occurring during LOCA & SGTR sequences, substantial progress has already been made and is detailed in this report. In addition to the modelling work and the improvement of the calculation chains, new experimental data and NPP measurements have also been made available to the partners (i.e. on clad H2 uptake, on iodine activity in VVER primary circuit…). Although delays in the realization of certain actions by some partners have been noted, this should not fundamentally impact the running of the project and jeopardize the completion of this work at the end of summer 2022.

In WP5 dedicated to innovation progress has also been made. The bibliographic work allowing to make the status in existing devices, Accidental Management Procedures (AMPs) and diagnostic tools worldwide, in the nuclear field but also more generally in the industrial field has been finalized and identification. Both identification of devices (including instrumentation) of interest and development of some algorithms for the improvement of AMPs have been already performed. Finally for the evaluation of Accident Tolerant Fuel, both identification/collection of thermo-physical/chemical properties and preparatory work on some of the simulation chains that will be used for their evaluation and the associated uncertainties/sensitivity analyses have been made.

In conclusion, the project is on track and no major and redhibitory deviations have been noted during this second year, in spite of highly disadvantageous conditions for the management and the cohesion of the whole group. The few delays observed should be able to be made up during the coming year.