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Abbreviations

AI	Artificial Intelligence
ANN	Artificial Neural Networks
ATF	Accident Tolerant Fuel
BEPU	Best Estimate Plus Uncertainties
BWR	Boiling Water Reactor
DBA	Design Basis Accident
DEC-A	Design Extension Conditions-A
ECCS	Emergency Core Cooling System
EPR	European Pressurised Reactor
EP&R	Emergency Preparedness and Response
FG	Fission Gas
FP	Fission Product
HBS	High Burn-up Structure
IAEA	International Agency for Atomic Energy
LB	Large Break
LOCA	Loss Of Coolant Accident
NEA	Nuclear Energy Agency
NPP	Nuclear Power Plant
PCC	Pearson's Correlation Coefficient
PRISE	PRImary to Secondary leak accident
PWR	Pressurized Water Reactor
RC	Radiological Consequences
RCS	Reactor Coolant System
RIA	Reactivity Insertion Accident
RPV	Reactor Primary Vessel
SA	Sensitivity Analysis
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

Primary motivation of the R2CA project is the increase of the NPP safety in Europe. To do so it is intended both to provide more realistic evaluations of 2 categories of DBA accidents and consider accidental situations more severe than those integrated in plant designs, i.e. the DEC-A conditions. The project will examine all these accidental scenarios through the prism of the prism of the radiological consequences

More especially, the main objectives of the R2CA project, dedicated to the Reduction of Radiological Consequences of explicit Accidents within design basis and design extension conditions (restricted to DEC-A) for Gen II, III and III+ Nuclear Power Plants, are:

- To consolidate/refine the 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 provide rationales/develop innovative measures, devices and tools for an earlier diagnosis of those accidents, for their management strategies and their mitigations.
- To provide guidelines for a harmonization of the methodologies used in Europe for evaluating their radiological consequences.

To meet these objectives several specific actions have already been performed or are in progress as:

- To make a review and collection of the existing experimental data useful for verifying and calibrating the updated/improved models and/or advanced simulations tools developed during the project for fission product behaviour and transport in the primary circuit, fission product releases from the fuel rods and fuel rod/clad behaviour during LOCA and SGTR accidental transients within DBA and DEC-A conditions.
- To 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 limits of the considered reactor models within DBA & DEC-A conditions, through the RC of LOCA & SGTR bounding scenarios.
- To provide advanced simulation tools and calculation schemes allowing to reduce the degree of conservatism and derive more realistic safety margins limits through the RC evaluation of bounding LOCA & SGTR 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 (i.e. PWRs, VVERs, EPR & BWR).
- 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: perform reactor calculations of both LOCA and SGTR bounding scenarios for DBA and DEC-A conditions and propose harmonized methodologies for the evaluation of their RC as a marker of increased safety in NPPs through more realistic evaluations of the safety limits.
- 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 (i.e. namely the number of fuel rod failures) and release/transport of fission products through the containment 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 (i.e. namely the increased activity in the primary coolant circuit) and release/transport of fission products through the defective steam generator up to the environment.

- WP5-INNOV: identify and evaluate the gains using the developed/improved 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 3rd 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 to 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, training on simulation tools and activities 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 finalized, and a preliminary analysis of their results performed. The tool intended for the evaluation of radiological consequences was also finalized. The calculation results were stored in excel file datasheets that should help to further create the expected database.
All this work was included in the deliverable 2-5 issued during the 3rd year of the project. This deliverable was slightly delayed mainly due to COVID-19 related problems and to a lesser extent to the war in Ukraine which also delayed the work of our Ukrainian colleagues.
In the meantime, following the work carried out in the WP3 & WP4, improvements were made in the modelling of the key phenomena involved in the release of fission product activities into the environment during LOCA and SGTR accidents within DBA & DEC-A conditions, as well as in the calculation methodologies used for their evaluation (couplings of simulation tools etc.). These updated calculations chains were used to start re-running the reactor test cases performed at the beginning of the project.
In the same way and for the same reasons, the work planned in the R&D WPs (i.e. in WP3-4 & 5) was also delayed and some R&D actions have been postponed. The corresponding final deliverables of WP3 and WP4 were then for the most part with the exception of one (delayed further) postponed from August 2022, date on which they were expected, to February 2023.

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

- **WP2**: The final report of T2.3 gathering the main outcomes of the first set of reactor calculations was issued (~ 48 scenarios LOCAs or SGTRs, DBA or DEC-A; 8 different reactor concepts including VVERs, PWRs, EPR and BWR-4). Corresponding excel data sheets gathering the main results (Thermal-hydraulics, thermo-mechanics, FP release kinetics…) were also completed. Meanwhile the second set of reactor calculations using the upgraded calculation chains (benefiting from WP3 & WP4 work) as well as updated evaluation methodologies for the FPR releases into environment were initiated.
- **WP3**: Additional clad burst models were implemented in some codes (i.e. DRACCAR, FRAPTRAN…) as well as model adaptation for mainly Zr-based alloy plastic deformation, high-temperature creep and crystallographic phase transition. At the same time, for a better prediction of the whole number of failed rods, refined approaches for the whole core description were elaborated (in DRACCAR and ATHLET-CD mainly) and the statistical methods tested. Improvements were made in some codes to better simulate the FG releases (i.e. from HBS in ASTEC/REL, ATHLET-CD). Meanwhile, a higher degree of mechanistic modelling was implemented in fuel performance codes (i.e. TU, FRAPCON) by their coupling with mesoscale codes describing the behaviour of FG/FP behaviour at the fuel grain level and their verification made upon different irradiation/transient tests. Some modifications were also implemented in COCOSYS regarding the FP (esp. related to iodine) behaviour in containment and some BEPU analyses performed.

Finally, the models for FP transport/in-containment behaviour were also re-assessed upon selected tests of the R2CA experimental database within the boundary conditions representative of DBA and DEC-A conditions.

- **WP4**: In order to better simulate the behaviour of fission product during a SGTR transient (esp. the volatiles), code capabilities were enhanced with new physic-based models, with external functions or user's driven coefficients (TRANSURANUS, SCIANTIX, MFPR-F, RING, MAAP, RELAP5, MELCOR, ASTEC). These developments covered I/Cs peak releases from fuel to gap-primary coolant and iodine transport from primary-to-secondary in the failed SG such as partitioning, steaming phenomena). For clad secondary hydriding also both simple models for H_2 uptake at low temperatures in Zircaloy-based materials and a multi-physical model in SHOWBIZ simulating all the phenomena from water ingress to hydride blister formation were developed.
- **WP5** A numerical optimization method for the timing of operator actions during a SGTR for VVER 1000 and PWR has been developed as well as a specific accident management strategy for PRISE in VVERs including the the automatic identification of the considered accident based on its inherent characteristics and the automatic start-up of the algorithm for accident control. Meanwhile, an innovative approach using Artificial Neural Network was developed to make predictions for clad defect detection. To this end, a new physical model for the fission product release and coolant activity calculation was developed to generate a computational database on which the ANN was further tested both against the activity of isotopes of interest in coolant and against the defect status. Finally, regarding ATFs extension of some fuel performance codes (DRACCAR, FRAPTRAN, TRANSURANUS) have been performed and some evaluations performed with the modified codes focussing on Cr-coated Zr4 clads and on U_3S_{i2} fuel and FeCrAl cladding. First results show that most of ATF technologies can delay the time and/or the temperature of cladding failures.
- **WP6:** Regarding dissemination a second newsletter was issued, the third prepared and eight R2CA related publications were issued that were published in journals or were presented in international/national conferences (NENE2022, NURETH19, ERMSAR22, Annual Meeting of the Spanish Nuclear Society,). A special issue on R2CA gathering open-access papers was also initiated. Regarding Education & Training a DRACCAR training course was organized gathering 15 participants from 7 different organisations participating to the project. Additionally, one mobility was completed and a post-doctoral initiated.

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 meets the project main and specific objectives and was consistent with the work originally planned by each of the consortium partner. A special attention has been paid to the reactor calculations for which some difficulties have been encountered.
During the third year, the main challenge of the management team, as for the second year, 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 second-year progress meeting was held remotely, gathering more than 50 European experts, researchers and students from the 17 organisations participating to the project, in September 2021. The meeting took place over 3

days; with a large part dedicated to the progress of the R&D work performed in WP3 and WP4 and their key reporting dates (**Erreur ! Source du renvoi introuvable.**). During this meeting, it was proposed to submit a common publication describing the general aspects of the project and the overall work progress made so far at the ERMSAR 2022 conference.
Regarding the financial aspects, it was mentioned that only 10% of the initial budget allocated to “Other direct costs” was at that time spent due to the COVID crisis (i.e. because of delay in mobility, cancellation of meetings and associated travels). In view of these observations, possible adjustments for the second or third period and potential cost reallocation were discussed.

In May 2022 was organized also remotely the 2nd Management Team Meeting gathering the work packages and task leaders. The objective of this meeting was to share technical information about the work progress since the last progress meeting at a key point in tile for WP3 & WP4 (i.e. 3 months before their expected work finalisation and their final report issuing) and identify any difficulties in partner’s work progress that could impact the task objectives and the overall project (incl. actions that might not be realized). During the meeting was also discussed the preliminary list of papers to be included in the foreseen special issue of “Annals of Nuclear Energy”.

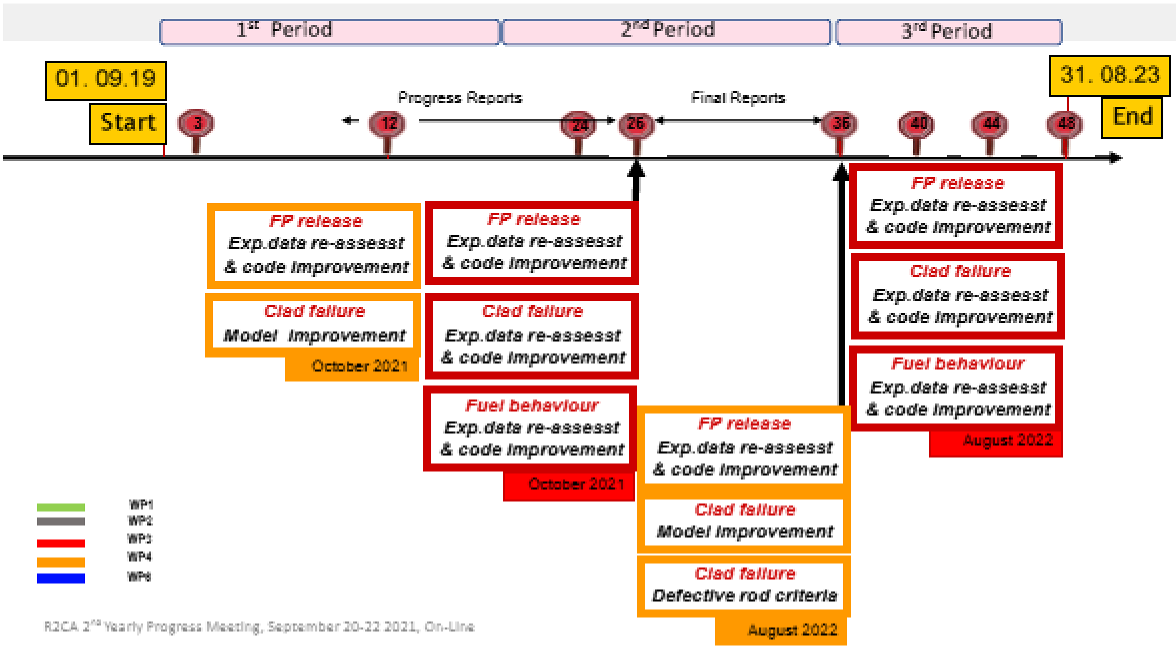

Figure 1: 3rd year deliverables

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, the first two ones have been completed during the first project period. First one consisted in performing three different reviews (on RC evaluation methodologies used in some of the countries participating to the project, on available experimental data relevant for the project and on the capabilities and models of the simulation tools planned to be used for LOCA and SGTR scenario under DBA and DEC-A conditions). This task, in particular, allowed to identify the major sources of uncertainties and gaps remaining in source term evaluation methodologies and simulation tools as well as the experimental data that will be useful for the validation or re-assessment of the models used for calculating the activity releases into the environment within DBA and DEC-A conditions in LOCA and SGTR scenarios. It served as a basis for proposals for model improvements. Within the second task, a simplified tool for the evaluation of radiological consequences in the scenarios of interest has been built and provided to the consortium in the form of an excel file.

During the third year of the project, the first set of reactor calculations were finalized, associated datasheets provided and corresponding analyses of the results performed. Some of the main results and outcomes were presented at the ERMSAR conference held in Karlsrühe in May 2022 and included in a paper recorded in the conference proceedings. The second set of calculations using the improved codes and calculation methodologies was also started using the same scenarios as for the first set of calculations. Furthermore, sensitivity analyses on key parameters and uncertainty quantifications were also initiated by some partners.

Finally work in Task 2.6 dedicated to the harmonisation of methodologies for radiological consequence evaluations following LOCA and SGTR transients within design basis and extended design conditions was started.

The specific objectives of the corresponding tasks (task 2.3, task 2.5 and task 2.6) for the time period considered are recalled below:

- 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 and provide the corresponding datasheets
  - Analyse the calculation results
  - Identify gaps in modelling/calculation methodology and propose ways for improvements
- Task 2.5 – The objectives for this task were:
  - Make a second set of simulations of the reactor cases using improved models and calculation chains/methodologies and provide the corresponding datasheets
  - Analyse the updated calculation results and quantify the obtained gains compared to the first set of calculations
  - Perform some sensitivity analyses and uncertainty quantification
- Task 2.6 – The objective of this task was:
  - To formulate best-practices for LOCA and SGTR DBA & DEC-A scenarios

To elaborate updated and harmonized methodologies for the evaluation and the reduction of radiological consequences in DBA and DEC-A conditions applicable to various operating reactor concepts in Europe

2.2.2 Overview of the main advances

In task 2.3 about 40 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. This was mainly accomplished during the second year of the project. Deliverable (D2.5) summarizing all these 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 has been issued during the 3rd year.

Datasheets gathering the overall results from this first set of reactor calculations were also completed during this 3rd year. Meanwhile, few datasheets were also already provided for the updated/improved calculation results performed within Task 2.5. In this latter task, experience gained in Task 2.3, plus models and methodologies improvements developed in WP3 and WP4 in order will be used to re-assess the calculation provided in first set of the calculations. As for the initial set of reactor calculations, the individual technical reports submitted by each partner involved in this task will be used for the summarising report (D2.7) expected during the last project period.

Based on the simulation results achieved in Task 2.3 and Task 2.5 as well as the outputs of WP3 and WP4, best-practices for more realistic reactor simulations for LOCA DBA, LOCA DEC-A, SGTR DBA and SGTR DEC-A conditions will be formulated and argued as well as harmonized evaluation methodologies proposed.

These activities have just started by summarizing the work performed so far in T2.1 regarding methodology review and in T2.3 summarizing the main reactor calculation outcomes.

2.2.3 Details of the activities performed

2.2.3.1 Task 2.3: Initial set of reactor calculations

The first set of reactor calculations was completed during the second year of the project and the corresponding technical reports issued.
As expected, due to differences 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 was performed during the 3rd year to explain those differences. Deliverable D2.5 where the main outcomes of these calculations, the modelling methods and approaches as well as the main hypotheses and assumptions used are given was also finalized during the third year of the project. It also highlights both the model development needs for a more realistic evaluation of the source term and model improvements that will be performed within Task 2.5.

The calculation results achieved in the Task 2.3 allowed to highlight where improvements in the simulation tools and modelling approaches could be made to better estimate the environmental releases during evaluated transients and then adjust the decision-making processes. These improvements initiated in July 2020 were mostly finalized during the 3rd project year. They can be roughly divided into four main categories:

a. Improvements of plant models (i.e. by updating approach of core modelling, upgrading nodalization);
b. Improvements of calculation chains and methodologies (i.e. by coupling of more mechanistic simulation tools, using statistical approaches for evaluating the number of fuel clad burst);
c. Improvement of computational models at different levels of details (i.e. by developing new cladding burst models better corresponding to the experimental data, by refining clad burst criteria, including user-driven correlations like iodine spiking modelling);
d. Developments/improvements of mechanistic modelling for a detailed modelling of important processes (i.e. fuel rod clad deformation and rupture, clad secondary hydriding, high burn-up structure growth and associated FP releases, FP releases from fuel rod gaps, atomisation, flashing processes in failed SG). These detailed improvements could help to improve the prediction of low-informed models.

As already mentioned during the 3rd year, all partners provided filled datasheets with results corresponding to the Task 2.3 calculation results and the final deliverable of the task was finalized. Task 2.3 is thus completed.
The table below summarizes all the calculations made.

Table 1: Status of the initial reactor test case simulations

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	
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	-	-

2.2.3.2 *Task 2.5: Reassessment of reactor test cases (quantification of gains)*

This task involves all partners who have already participated in the Task 2.3, using their gained experience as well as the improvements made within WP3 and WP4 (relating to models, calculation chains & simulation methodologies). It consists in recalculating the same scenarios as in task 2.3 in a less conservative manner by using the improvements made.

During the 3rd year of the project, several videoconferences were organized (on March 9th, 10th, 11th, 15th and then later on August 25th and September 8th) in order to share the progress in Task 2.5 work and to further discuss the possible improvements for LOCA and SGTR accident scenarios calculations that could be beneficial especially for partners who were not involved in WP3 and WP4 developments. During these meetings were thus discussed the planned improvements for each calculation, their foreseen improvements as well as the needs and inputs to be shared amongst partners. The results of the above-mentioned meetings are summarized in the **Erreur ! Source du renvoi introuvable.** and **Erreur ! Source du renvoi introuvable.**. During the last two meetings, it was also discussed how to best manage the delays of some partners in the realization of the calculations leading to a postponement by about 6 months of the final report of this task (deliverable D2.7). The current progress and planned individual report submission date of each partner are presented in **Erreur ! Source du renvoi introuvable.**. Finally, during these last meetings partner's intent in terms of sensitivity analyses and/or uncertainty evaluation for both kinds of scenarios were also shared and discussed (**Erreur ! Source du renvoi introuvable.** & **Erreur ! Source du renvoi introuvable.**).

Table 2: Planned activities in Task 2.5, LOCA scenarios

Participant	Planned improvements	Calculation chain	Needs/Inputs from partners, Possible collaboration
IRSN	Improvements of the cladding rupture correlations and FG release models.	FRAPCON/ DRACCAR/ SOPHAEROS	With ENEA with new burst
ENEA	The accuracy on the estimation of failed rods number is closely interconnected to the modelling of core thermo-mechanical behavior which is one of the main points to be improved.	ASTEC	Support of IRSN to define a map of power/FPs distribution detailed enough for the new foreseen core modelling which implies a high number of representative fuel rods.
ARB	Thermal-mechanical analysis was not performed. Very conservative assumption for FP behavior, and it is planned to be changed in the work related T2.5. Calculation time for some cases need to be extended.	COCOSYS	UJV - with COCOSYS models SSTC, UJV, EK - with fuel failures.
LEI	Estimation number of failed rods and the accuracy of such a prediction	ASTEC/ TRANSURANUS / ASTEC	No
VTT	Improve the LOCA cladding failure capabilities of the single rod fuel performance code FRAPTRAN.	FRAPTRAN	Possible with IRSN and EK
EK	It was considered that FP from the fuel released to the primary coolant instantaneously. This is very conservative assumption, and it is planned to be changed in the work related T2.5.	FRAPTRAN	No
HZDR	Very conservative assumption for FP behaviour, and it is planned to be changed in the work related T2.5.	ATHLET-CD	No
UJV-NRI	Very conservative assumption for FP behaviour, and it is planned to be changed in the work related T2.5.	ATHLET/ TU/ COCOSYS	Possible with ARB regarding COCOSYS improvements
SSTC_NRS	Thermal-mechanical analysis was not performed. Very conservative assumption for FP behaviour, and it is planned to be changed in the work related T2.5. Calculation time for some cases need to be extended.	RELAP/ TU/ MELCOR or RELAP/ MELCOR	Collaboration with ARB regarding the fuel cladding failure evaluation.

Table 3: Planned activities in Task 2.5, SGTR scenarios

Participant	Planned improvements	Calculation chain	Needs/Inputs from partners, Possible collaboration
IRSN	Implementation of correlations for Iodine flashing/partitioning in the affected SG. Iodine/release calculations with MFPR-F/TU and improvements of iodine spiking models in SAFARI.	ASTEC/ SAFARI	No
BOKU	Evaluation of the radiological consequences in the vapor phase (limitation of RELAP5-3D). Implementation of iodine spiking model for the RELAP5-3D. Accident management strategy improvement.	RELAP5-3D 4.0.3	Need help for data for generic model. Will prepare the list of the needed data. Possible with NINE
ARB	Reducing the conservatism of the release into the environment by taking into account the mixing of the primary coolant (its activity) with the ECCS water. Optimization of emergency operator actions.	ATHLET3.2	Need help from colleagues to reduce the conservatism in the assumptions in the primary part.
Bel V	CATHARE capabilities to model the spiking phenomenon and the transport of radiochemical elements will be assessed.	CATHARE2/ V2.5_3/mod8.1	Possible with POLIMI and CIEMAT
TRACTEBEL	Improvement of the partitioning model. Direct modelling of spiking by MELCOR2.2.	RELAP5 mod2.5 MELCOR2.2	Possible with CIEMAT.
EK	Determination of maximum activity concentration in the primary coolant. Iodine spiking effect simulation Evaluation of the activity released to the environment.	RELAP5mod3.3 COSYMA code	No
UJV-NRI	Modification of the existing model for ATHLET-CD calculations, which offers fission product transport calculated tightly with the TH calculation using the sophisticated SOPHAEROS module. Extension of the calculated fission products in accordance to the JRODOS computational capability.	ATHLET3.1	Need help for new approach for SGTR analysis to reduce conservatism.
SSTC_NRS	Consider mixing coolant with ECCS water to estimate the portion of contaminated primary water discharged to environment. Consideration of the decay of radioactive isotopes with time. Improvements in the primary side to reduce conservatism.	RELAP5mod3.2	Possible with ARB
CIEMAT	Develop a control function that enables partitioning of iodine between water and gas. To enhance the iodine spike modeling used for T2.3. Iodine handling in its transport from RCS to the gas phase of the secondary side in the failed SG.	MELCOR2.2	Possible with TRACTEBEL

Table 4: Status of individual reports and datasheets to be provided in Task 2.5

Organization	Type of reactor	LOCA		SGTR	
		DBA	DEC-A	DBA	DEC-A
ARB	VVER-440;	NOT received Planned Mid of February	NOT received Planned Mid of February	NOT received Planned Mid of February	NOT received Planned Mid of February
	VVER-1000	NOT received Planned Mid of February	NOT received Planned Mid of February	NOT received Planned Mid of February	NOT received Planned Mid of February
Bel V	PWR-1000			NOT received End of February	NOT received End of February
BOKU	PWR-1300,			NOT received Beginning of February	NOT received Beginning of February
	VVER-1000			NOT received Beginning of February	NOT received Beginning of February
CIEMAT	PWR-1000			NOT received End of February	NOT received End of February
EK	VVER-440	Report received, Datasheets received RC evaluation not applicable		Report received, Datasheets received	
ENEA	PWR-900	Report received Datasheets received	Report received Datasheets received		
HZDR	PWR-Konvoi	NOT received End of March	NOT received End of March		
IRSN	PWR-900	NOT received, End of February	NOT received, End of February	NOT received, End of March	
LEI	BWR-4		Report submitted		
SSTC-NRS	VVER-1000	Report received, Datasheets received	Report received, Datasheets received	Report received, Datasheets received	Report received, Datasheets received
TRACTEBEL	PWR-1000				NOT received Mid-February
UJV-NRI	VVER-1000	Received RC evaluation is not done Mid of February		Received RC evaluation is not done Mid of February	
VTT	EPR-1600	Report received RC evaluation and Datasheets not applicable			
	VVER-1000				

Table 5: Sensitivity Analyses and Uncertainty Quantification planned for LOCA scenarios

	LOCA	
Case study for parametric sensitivity	ARB	Done in T2.3; Planned in T2.5
	SSTC-NRS	Ongoing in WP3 tasks
	UJV-NRI	Done in T2.3
	ENEA	Done in T2.3; Planned in T2.5
	HZDR	Done in T2.3
	IRSN	Done in T2.3; Planed in T3.2
	VTT	Done outside the project, planed in T3.2
	LEI	Done in T3.2
Uncertainty quantification		
	UJV-NRI	Ongoing in T2.5
	HZDR	Planning in T2.5, depending on work progress
	LEI	Done in T3.2

Table 6: Sensitivity Analyses and Uncertainty Quantification planned for SGTR scenarios

SGTR			
Case study for parametric sensitivity	ARB	Done in T2.3; Planed in T2.5	
	SSTC-NRS	Ongoing in T4.1	
	BOKU	Ongoing in T4.1	
	TRACTEBEL	Done in T2.3	
	BelV	Ongoing in T2.5?	
Uncertainty quantification			
	BOKU	Ongoing in T2.5	Cooperate with NINE

2.2.3.3 Task 2.6: Updated harmonized methodologies

The status of this task was presented during the 3rd Yearly Progress Meeting on 20/09/2022.
Deliverable 2.8 consists in a kind of overview of the whole project, summarizing main deliverables, performing links between them and also a critical review as far as possible.
Therefore, it's redaction began early in the project, at the same rhythm as issued deliverables on which it is based.

It's structure, including current progress, is organized in the following way:
- Summary of D2.1 "Review of the RC evaluations methodologies": already done at the end of 2022
- Reactor test cases (based of D2.5): already done
- Models and code improvements: started
- Final cases: not yet started

Conclusions (including critical review): not yet started

2.3 WP3-LOCA

2.3.1 Objectives

This Work Package aims to improve the different simulation tools and models used to analyse the LOCA transients and to evaluate their corresponding releases into the environment. It is focussed 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 up to the environment.
Its main objectives are to develop the knowledge and the accurate evaluation tools/models for better evaluate the activities released into the environment following Loss Of Coolant Accidents within DBA and DEC-A domains. To that extent, existing databases and models have been revisited and the existing codes used by the partners within the project were updated (enriched with new models). The performed code improvements dealt both with 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 by UJV)
- Task 3.2: Evaluation of failed rod number (lead by IRSN)

Task 3.3 Fuel rod behaviour during LOCA transient (lead by JRC).

2.3.2 Overview of the main advances

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

- Regarding the fission product transport and release, a review of the ATHLET-CD models was performed and new release coefficients implemented, new models were developed in SCALE for VVERs fuel and in APROS system code for aerosol gravitational sedimentation, a re-assessment of ASTEC-REL and ASTEC-TR was completed on some of the most relevant tests included in the R2CA database focussing on iodine transport in RCS and behaviour in containment, meanwhile an optimisation of fuel grain parameters in ASTEC-REL for better evaluating the high burn-up fuel releases was proposed from statistical studies, finally some BEPU analyses on iodine release from sump was also performed with COCOSYS.
- Regarding the evaluation of failed rod, additional burst models were implemented in DRACCAR and the code capabilities were extended to whole core description, an application was proposed with an eighth of the core modelled, a detailed core model was developed in ATHLET-CD using a full 3D thermohydraulic modelling of the RPV and core, several modifications were proposed by different partners in FRAPTRAN (refitting of the plastic deformation model for E110 clad, two high-temperature creep laws for Zircaloy and M5 to be used in combination with a dynamic crystallographic phase transition model) and different burst criteria were implemented and tested against experimental data, in TU the implementation of the crystallographic phase transition model and creep law for M5 was finalised, sensitivity studies were also performed with ASTEC, an different approaches for the whole failed rod number in the core using TU (multistage, statistical) were used.

Regarding the fuel behaviour during LOCA transient, a higher degree of mechanistic modelling was implemented in fuel performance codes (FRAPCON code was coupled to SCIANTIX, TU/MFPR-F coupling completed with inclusion of feedbacks to TU), a service module was developed for off-line interface between TU and reactor dynamics and thermal-hydraulics codes, the development of the stand- alone module for axial gas communication during a LOCA coupled to creep models was completed, FG models in codes have been refined (HBS models in MFPR-F, a prior error control in SCIANTIX), an alternative NORTON creep law and clad failure limits were introduced in FRAPTRAN. All these improvements were verified and validated upon selected experimental tests (3 transient and 3 irradiation tests. Finally, uncertainty and sensitivity analyses with TU using a Monte-Carlo approach were also performed.

2.3.3 Details of the activities performed

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

The main objective of the task 3.1 for the third year was to improve the code abilities and to summarise the work conducted. The achieved progress was presented at the meeting in Bologna by all partners.

In the framework of the task 3.1, ENEA performed a review of the validation of ELSA module of the ASTEC code, focusing on the release of fission products and structural materials in conditions expected for LOCA DBA and DEC-A transients, i.e. with high burn-up and low temperatures. In particular, the VERCORS experimental program, through the RT1 and RT6 experiments, provided data for the optimization of the grain parameters of the ELSA module. The two experiments were simulated with an input deck provided by IRSN and the experimental data regarding the FP gas releases were compared to the ASTEC results. 1000 calculations per experiments were performed with a random selection of the parameters of interest (i.e. NCLG, SIGM and DGRA). The optimized values for these parameters were evaluated, following an optimization criterium that assesses the minimum value of the quadratic difference between the ELSA results and the experimental data. Reasonable agreement with the experimental data was achieved.

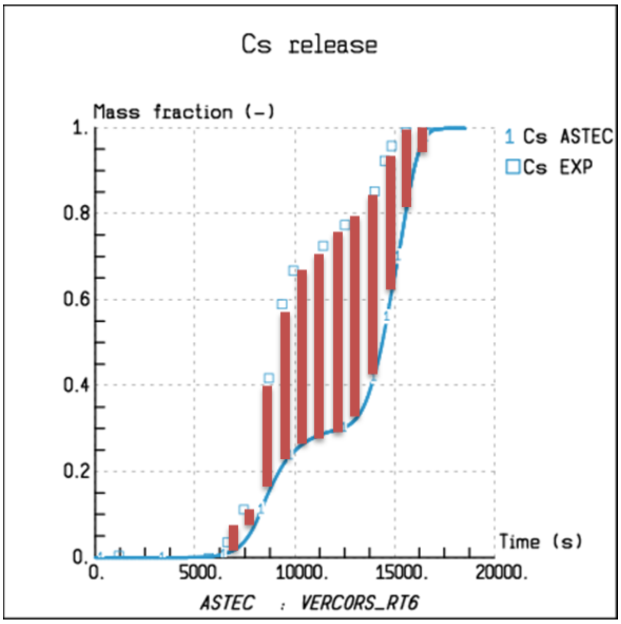

Figure 2: Experimental and simulated Cs release in VERCORS RT6 experiment, along with the integral to be optimized.

HZDR has reviewed the fission product release models implemented in the ATHLET-CD code with a focus to the phenomena important to DBA LOCA. The review was supplemented by ATHLET-CD analyses for a generic German PWR of type Konvoi (Siemens KWU design). For this purpose, the code has been extended, that the user can apply uncertainty factors for the release of selected elements separately.
It was found that the release rates (based on experimental data published by ORNL [Lorenz, 1985]) do not play a significant role for DBA LOCA. The main releases originate from the fission products accumulated in the fuel rod gap. However, ATHLET-CD does not model the process of accumulation, but instead applies a burst release model based on experimental data. Three different burst release models are implemented. The model based on the CORSOR code [Kuhlmann, 1985] has been investigated in more detail and uncertainty factors originating from analyses reported in the Reactor Safety Study (WASH-1400) have applied [USNRC, 1975]. It was found that these uncertainty factors are too high and new release coefficients based on the Draft Regulatory Guide DG-1389 [USNRC, 2022] have been implemented as alternative.
Furthermore, the ATHLET-CD input data set for the generic Konvoi has been extended by modelling also the transport of fission products within the primary circuit from the core to the break and some test calculations have been done to improve the estimation of activity accumulated in the containment.

IRSN contribution aimed at ASTEC code development. The models of ASTEC-TR module (i.e. SOPHAEROS module) dealing with FP behaviour during their transport in the primary circuit and the reactor containment, which were initially validated for what concerns iodine against a reference database mostly dedicated to severe accident (Phébus-PF, ISTP, OECD/STEM), were reassessed by IRSN to verify their applicability to LOCA DBA and DEC-A conditions.

Considering the containment dose rate and temperature encountered in the simulations of LOCA DBA and DEC-A for PWR-900 reactor performed in Task 2.3 as reference conditions of such accidents, three tests of the ASTEC validation database have been found to comply with these conditions:

- STEM/EPICUR LD tests for inorganic and organic iodine releases from Epoxy paint under irradiation (**Erreur ! Source du renvoi introuvable.**).
- the G1 test from the BIP program for interaction of gaseous inorganic iodine with dry stainless steel.
- the Iod9 from the THAI facility for iodine mass transfer and adsorption on steel wall.

The re-assessments of these tests show a reasonable agreement of the ASTEC-TR model previsions with the experimental data thus showing at the same time the applicability of the models for the DBA & DEC-A conditions.

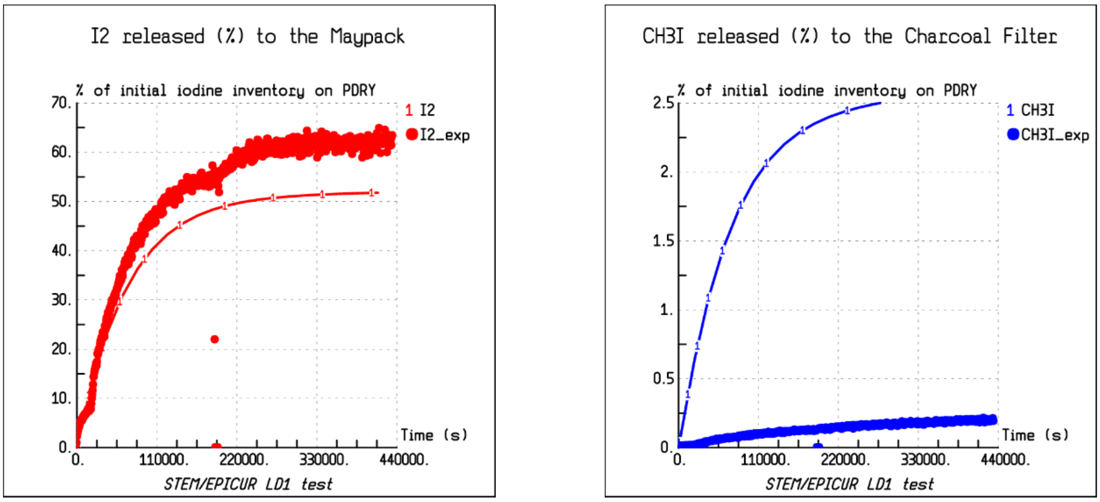

Figure 3: Re-assessment of Inorganic and organic iodine release during EPICUR LD1 test with ASTEC-TR

Regarding the ASTEC-TR validation grid for models in the primary circuit, the GAEC experiments performed in the CHIP facility and consisting in the transport of iodine down a temperature gradient from 1600°C to 150°C is found to be relevant in the context of DBA/DEC-A LOCA accident. Indeed, considering that the ASTEC/SOPHAEROS models were developed on a physical basis, they remain valid on the smaller temperature range encountered during LOCA accident.

SSTC activities were aimed at development of best-estimate models of the SCALE software package for the selected representative types of fuel assemblies used in WWER-1000 reactors of Ukrainian NPPs.
With use of the developed models the best-estimated source term for LOCA radiological consequences analysis was evaluated. As a result, the relevant knowledge on WWER-1000 fuel characteristics and its evolution characterization during in-core irradiation is enhanced. It gives possibility to decrease level of conservatism of assessment of LOCA radiological consequences.

VTT is developing new severe accident models for its system code APROS. While the code has been extensively used for analysis of design-basis accidents, the severe accident models of APROS have been limited to VVER-440 reactors, and they have not had many active users. The goal is now to extend the capabilities of APROS from design-basis accidents towards more severe cases, applicable to all light water reactors. While the code development is done with VTT's own funding, in R2CA Task 3.1, a validation calculation of the gravitational deposition of aerosols was performed. The AHMED (Aerosol and Heat Transfer Measurement Device) experiment was chosen as the validation case. The calculated aerosol concentration in the air was compared to the measurement results (**Erreur ! Source du renvoi introuvable.**). The same test was also calculated with the MELCOR code. Both codes overestimate the aerosol concentrations, i.e. they underestimate the deposition rate. However, the MELCOR result is slightly better than the APROS result. The difference is partly explained by the agglomeration model, which MELCOR has, but it has not yet been developed for APROS. The agglomeration of small particles increases their deposition velocity. The APROS validation result can be considered satisfactory, and it is expected to improve when the agglomeration model is added in the future.

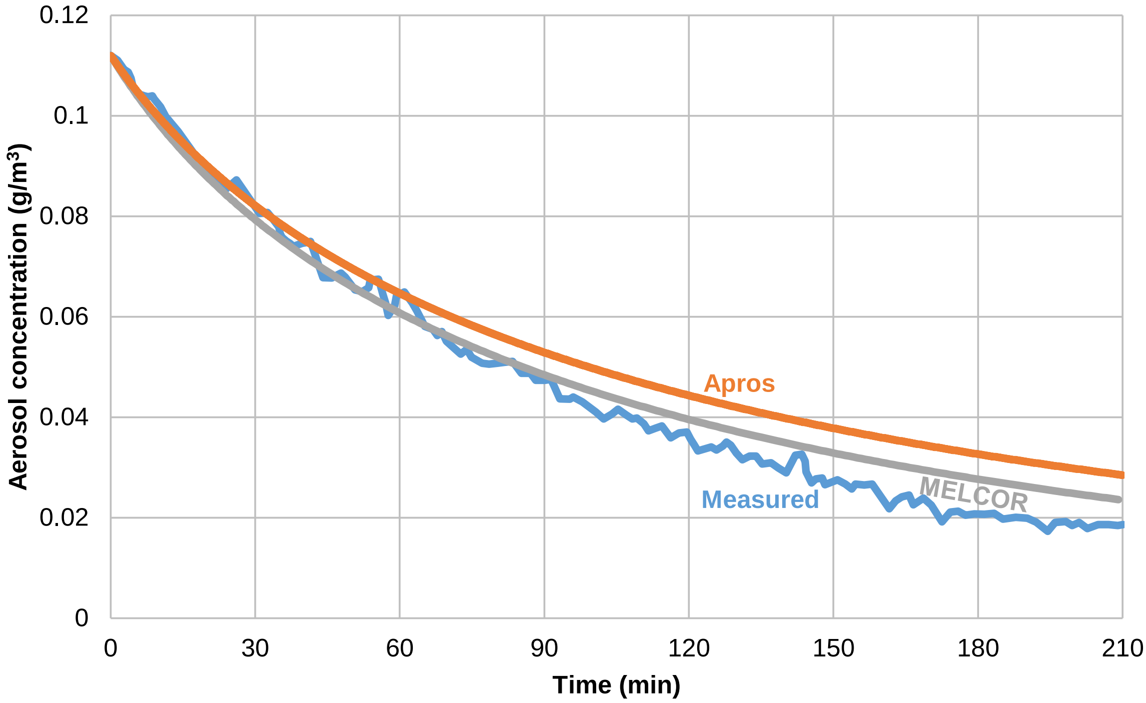

Figure 4: Aerosol concentration in the AHMED test, measurement compared with APROS and MELCOR calculations.

UJV further extended the validation work conducted in the previous years. The validation activities aimed at reassessment of the BIP experimental programme, namely the RTF test facility. This experimental series was described in the experimental database. The achieved results brought satisfactory agreement with the experiment. The information gathered in the validation was then applicated to sensitivity study of VVER-1000/V320 containment, where effect of the sump pH on the total iodine release for different initial iodine chemical composition distribution was studied. The results of this sensitivity study were presented at the 31st NENE conference in Portoroz, Slovenia. The containment related activities were further extended to a reassessment of initial and boundary conditions of a large break LOCA at VVER-1000/V-320. An extensive review aimed at external and internal initial and boundary conditions. The scope of the activities aimed at iodine release mainly. The GRS BEPU methodology and Spearman's correlation ratio were used to investigate the impact of the varied initial and boundary conditions and to estimate spread of the results (**Erreur ! Source du renvoi introuvable.**). Finally, UJV provided overall coordination of the task and participated in scheduled meetings.

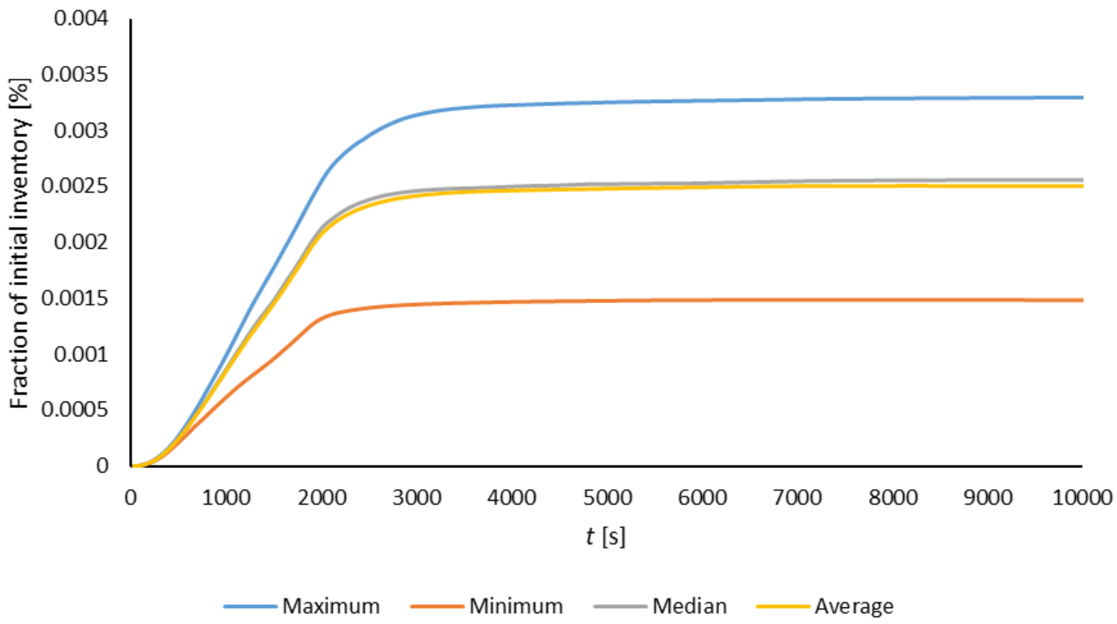

Figure 5: Results of the BEPU analysis of iodine release from VVER-1000/V-320 during LB LOCA (COCOSYS calculation)

References

M.R. Kuhlmann, D.J. Lehmicke, R.O. Meyer, "CORSOR User's Manual", NUREG/CR-4173. 1985, Battelle's Columbus Laboratories.

R.A. Lorenz, M.F. Osborne, "A summary of ORNL fission product release tests with recommended release rates and diffusion coefficients", 1995, Nuclear Regulatory Commission.

US NRC, "Reactor Safety Study", WASH-1400, 1975.

US NRC, "Alternative Radiological Source Terms for Evaluating Design Basis Accidents at Nuclear Power Reactors", Draft Regulatory Guide DG-1389, 2022.

2.3.3.2 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. It comprises updating/developing models for clad burst rupture and new approach for core modelling. Partner's contributions to task 3-2 during the 3rd year were mainly related to the finishing of the work performed during the second year and contributing to the final report.

IRSN work during last year was dedicated to finish the identification/verification/validation of burst criteria and DRACCAR new modelling for whole core simulations.

New Chapman type models on engineering burst stresses limited to as-received cladding were proposed (see **Erreur ! Source du renvoi introuvable.**) in complement to criteria proposed during the second year of the project. This model was then tested in the DRACCAR code on validation test cases not used in the identification data base.

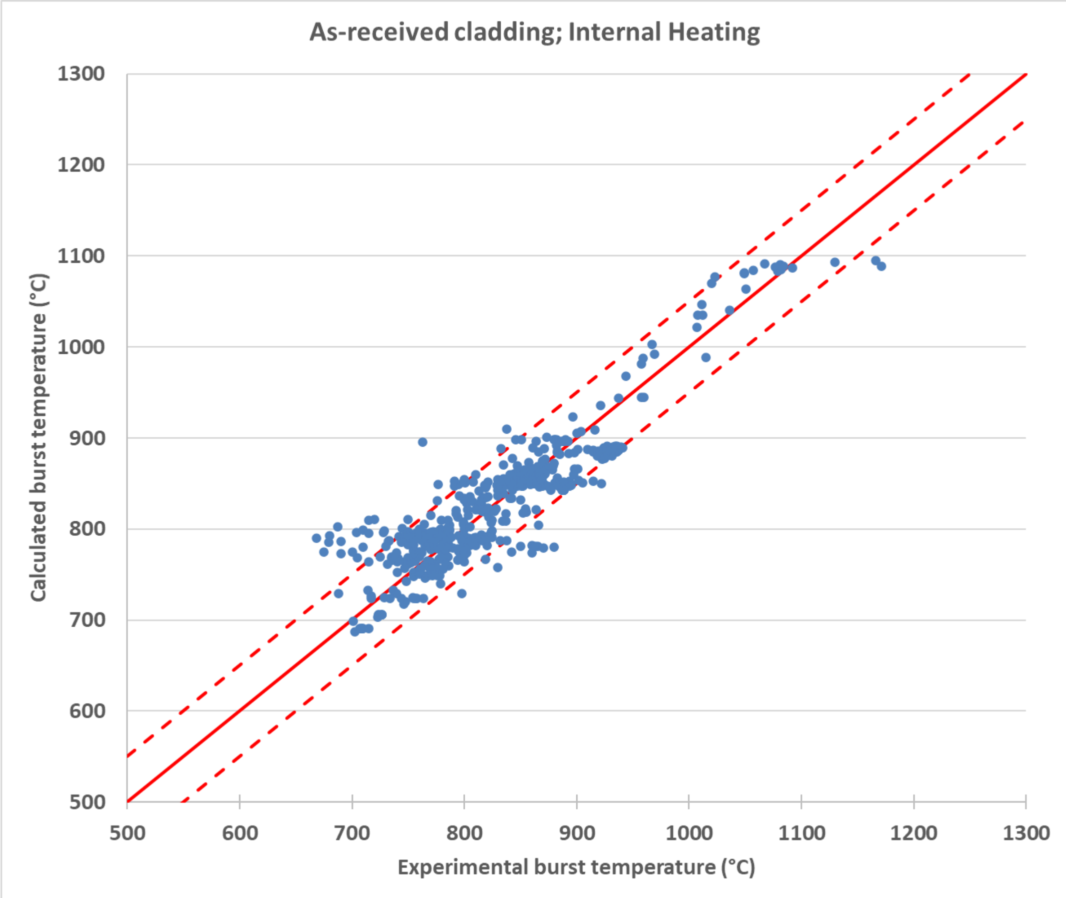

Figure 6: Calculated versus experimental burst temperature with the criterion on engineering stress. Doted lines correspond to ±50°C from the bisector line.

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 equivalent rods. In the frame of R2CA, DRACCAR capabilities were extended to the description of the whole core coupled to reactor primary and secondary loops. Due to compromise driven by CPU cost of 3D simulations (**Erreur ! Source du renvoi introuvable.**), the retained approach mixes several applications: one at the scale of the core possibly completed by other detailed analysis of fuel assembly at sub-channel scales (and based on thermohydraulic conditions derived from core simulation). Indeed, the performance of DRACCAR software are not consistent with simulating in few days a LOCA since running a large panel of simulation is required to feed uncertainty analysis for a given LOCA scenario.

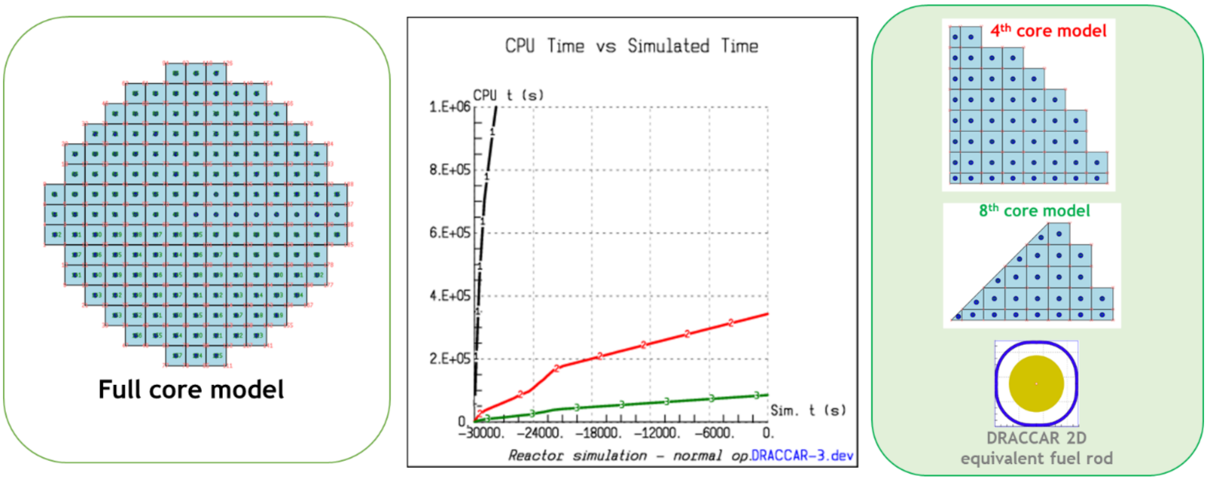

Figure 7: Cut view of DRACCAR core meshing with 2D equivalent fuel rods and associated CPU cost.

The main DRACCAR application proposed in new approach consists in representing a fraction of the core modelled using one equivalent rod per fuel assembly (900MW PWR uses typically 26 fuel channels to describe the eighth of the core). In this application, eighth of the core is coupled to the full RCS modeling (primary and secondary sides). Such simulation is able to depict the average behavior of fuel assembly accounting for fuel rod specificities (fuel type, burn-up, initial state, location in core) coupled to a thermal hydraulics description of the whole primary and secondary circuits at the system scale.

Meanwhile to methodology development, it was demonstrated from simplified case studies that:

- The equivalent rod model cannot depict the respective behavior of each fuel rods among a fuel assembly. The preliminary conclusions deduced from these 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 (**Erreur ! Source du renvoi introuvable.**). 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. As a consequence, the relevant scale to assess such scattering of response should be the “sub-channel” scale.

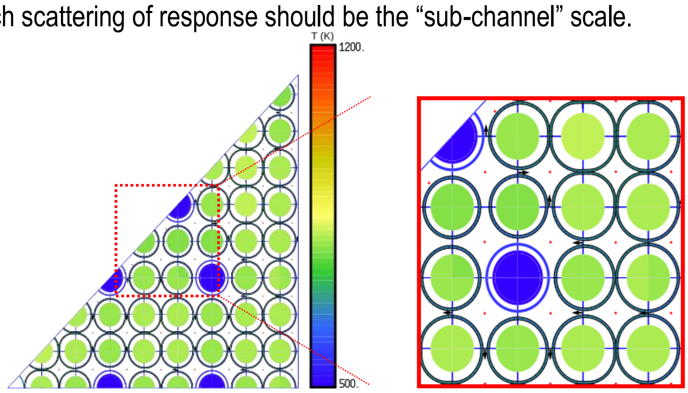

Figure 8: Thermal field and rod deformations simulated with DRACCAR 3D detailed PWR 17x17 fuel assembly model highlighting cold region close to guide tubes and non-symmetrical balloon contour.

- The interactions between a fuel assembly and its neighbors during a LOCA is mainly carried by transverse flow distribution (**Erreur ! Source du renvoi introuvable.**). No significant heat-up of the rods from the coldest fuel assembly was observed at the direct boundary with hottest fuel assembly. Therefore, from this case, it seems that interaction between fuel assemblies could be mainly represented using a 3D fluid model able to compute flow redistribution.

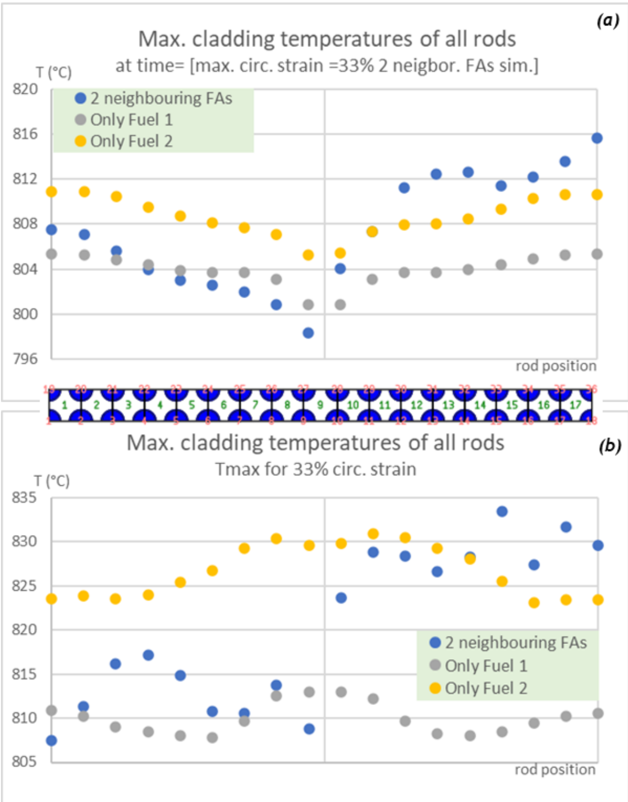

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Figure 9: PCT for each rod obtained when max circumferential strain 33% is reached for first time by one rod *(a)* PCT for each rod when rod circumferential strain is 33% *(b)*

From analysis of these case studies and as the computational performance of DRACCAR doesn't allow to describe each rod of the core at the sub-channel scale, the methodology proposed is to complete DRACCAR "core+RCS" simulation by complementary fuel assembly stand-alone simulations. These complementary simulations could provide insight on the fuel rod behavior using fined 3D assembly description at sub-channel scale based on average fuel assembly thermal hydraulics conditions derived from the "core+RCS" DRACCAR simulation. The specific modelling of this complementary studies mainly consists in an eighth of fuel assembly for which each rods (fuel rod, guided tubes with/without absorber, instrumentation tube) are modelled in 3D(r,θ,z) within a DRACCAR domain coupled to thermal-hydraulic domain at sub-channel scale closed by boundary conditions (from core+RCS simulation).
The proposed methodology by IRSN is schematically summarized on **Erreur ! Source du renvoi introuvable.** below. Of course, such methodology should rely on models at the state-of-the-art for LOCA analysis and should use suitable burst criteria model to assess the burst risk (such as the one recommended by IRSN in the frame of R2CA).

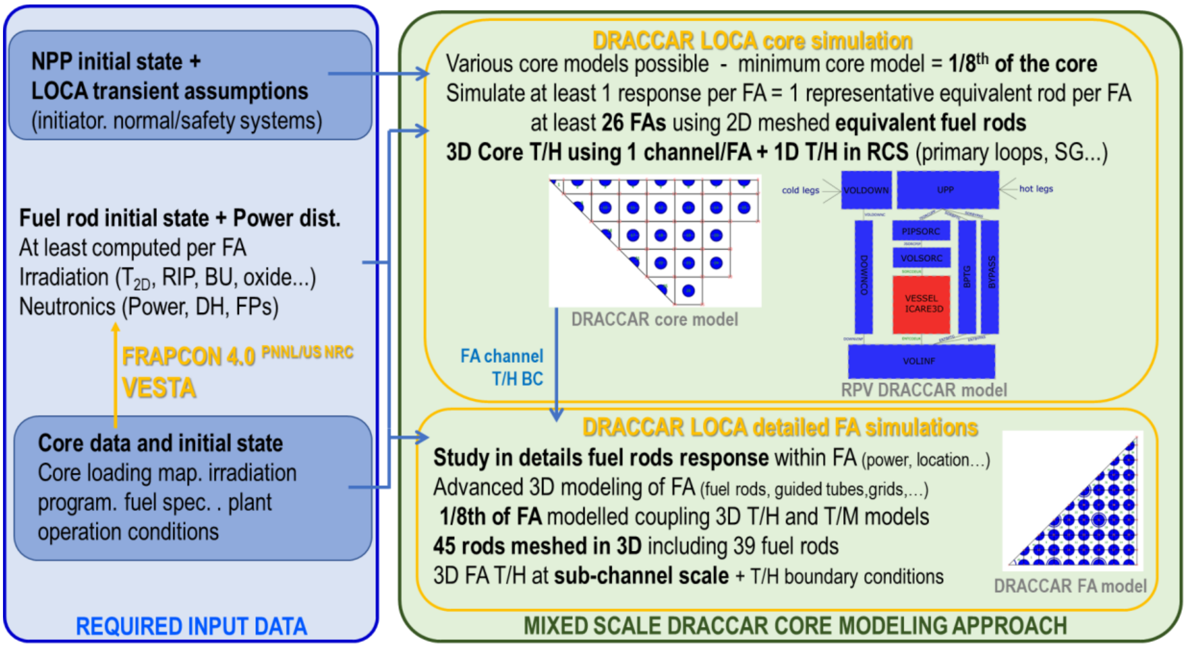

Figure 10: DRACCAR new core modelling approach to evaluate the number of failed rods during LOCA for LWR developed in the frame of R2CA project.

The development of DRACCAR core methodology was accompanied by developments such as improvement of the 2D equivalent rod model (for contact between rods description) and automatic procedure for fuel rod initialization (both using VESTA depletion code results and FRAPCON 4.0 fuel performance simulations) or core meshing.

As a conclusion of this year, the new "core+RCS" DRACCAR application was illustrated through a demonstrative simulation in the frame of task 2.5. This work shows that the method represents more realistically the fuel assemblies and their interaction with the rest of the core. Therefore, it's expected an improvement of the evaluation of the number of failed rods. Of course, the work proposed in the frame of project is a first step that led to identify prospects for the use of DRACCAR to predict failed rod number in LOCA conditions. One of the most important is to improve the computational capabilities by reducing the CPU cost of 3D core thermal hydraulics resolution. This will allow to extend domain from an eighth of core to a full 3D core description. Then it could be coupled to 3D RPV model and consider the non-symmetric flow distribution in core channels occurring in LOCA (and associated to the angular location of the connection between vessel and broken primary loop).

In the frame of the third year of R2CA, ENEA, in strict coordination with JRC, has finalized the review on M5™ models. Results of this review have suggested to consider in more detail the model published by Massih and Jernkvist for the crystallographic phase transition [Massih, 2021] (see **Erreur ! Source du renvoi introuvable.**) and a combination of Kaddour's and Massih's models for the high temperature creep [Kaddour, 2004] and [Massih, 2013]. These models have been implemented in the TRANSURANUS subroutines for verification by means of a standalone program. Additional considerations on Zircaloy-4 crystallographic phase transition have permitted to propose a preliminary modelling. Results of this activity have been presented at the NENE2022 conference [Calabrese, 2022]. These models will be tested against current TRANSURANUS modelling of LOCA transients.

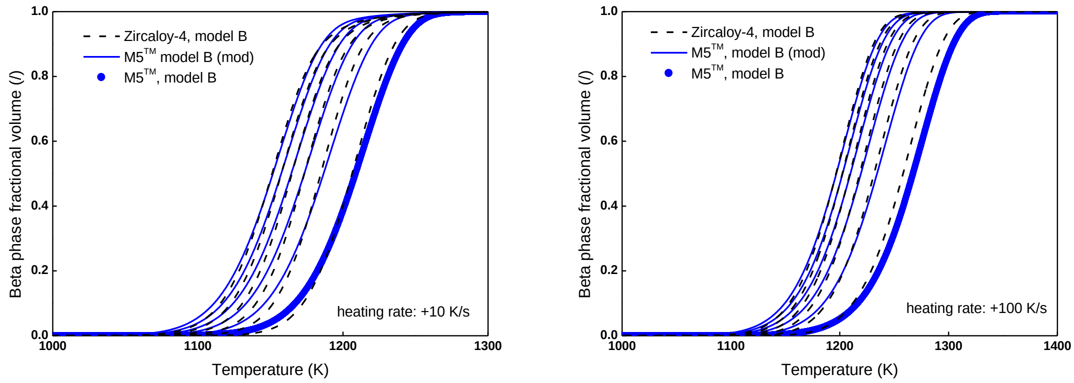

Figure 11 : Phase transition with concentrations of hydrogen in the interval 0-500 ppm (every 100 ppm): comparison of models at +10 K/s (left) and +100 K/s (right)

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 was to study the geometry of samples of the Russian alloy E110 that underwent ballooning and burst tests (see **Erreur ! Source du renvoi introuvable.**). In the third year of the project, new burst criteria have been established and using these new criteria the parameters of the cladding plastic deformation model of the code FRAPTRAN were re-fitted.

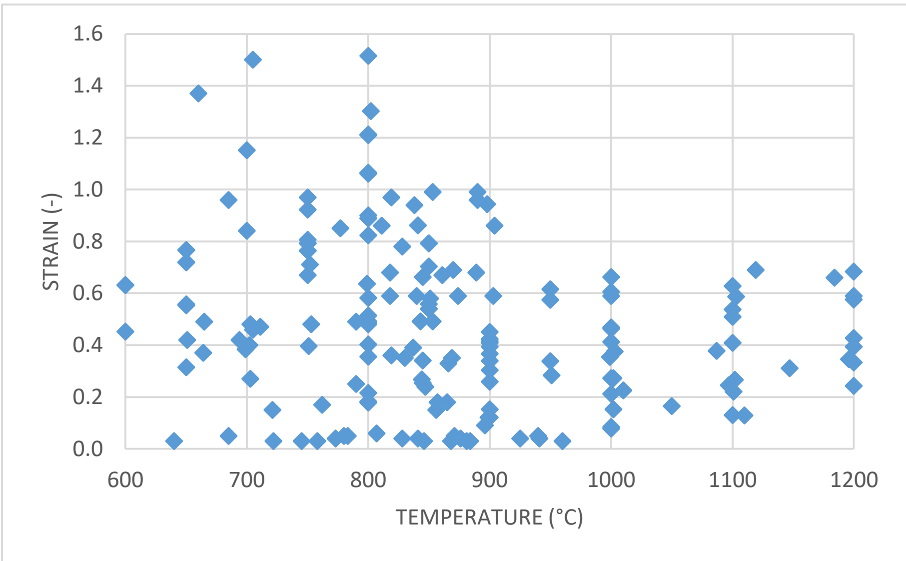

Figure 12. Available cladding burst strains from EK work

HZDR work during the 3rd year was dedicated to continuing the development of a detailed core model in ATHLET-CD (part of the AC^2 code package). A new core modelling approach has been developed which combines a 3D thermal hydraulic model of the PWR RPV and reactor core with the fuel rod model of ATHLET-CD (including mechanical rod behavior model, models for burst of cladding, calculation of fission product inventory and decay heat) and feedback from the fuel rod model back to thermal-hydraulic model (based on calculation of reduction of the flow cross sectional areas).

Despite the model still has several limitations and short-comings, it is (to the author's knowledge) the first time that the system code ATHLET-CD has been applied to model the degradation of fuel rods for a 3D configuration of PWR core. In contrast to the very coarse nodalization approach applied at the beginning of the project (subdivision of the core into 6 concentric rings, which is the typical approach applied in severe accident codes), the new approach enables to study the influence of local variations of the flow and cooling conditions to the behavior of the fuel rod (see **Erreur ! Source du renvoi introuvable.**). This is especially important for the analyses of a LB-LOCA with asymmetric boundary conditions due to break located in only 1 out 4 loops and asymmetric ECCS injection. With the new model the number of burst fuel rods during the LB-LOCA accident could be estimated, which was not possible with the previously used approach.
To investigate the performance and the capabilities of the new model, several LB-LOCA transients have been calculated for a generic German PWR of type Konvoi, with variation of the boundary conditions as well as model parameters and the number of failed rods has been calculated.

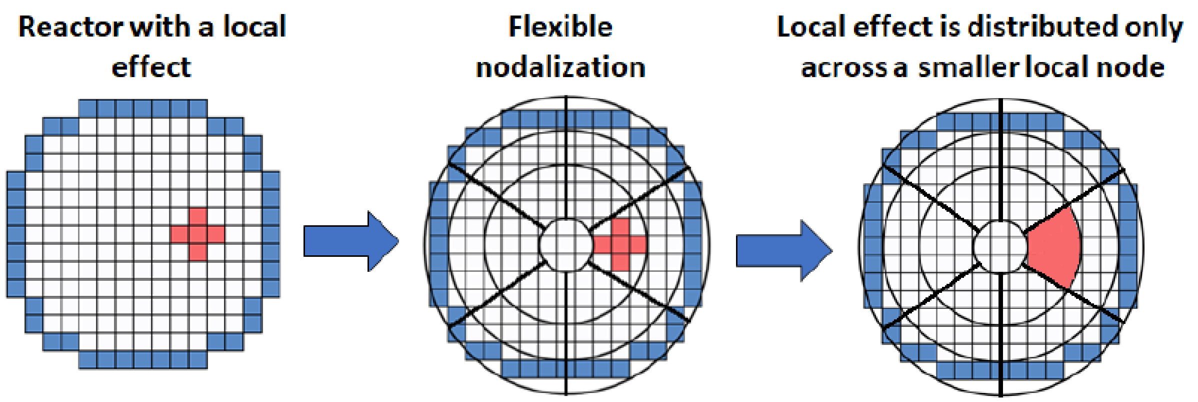

Figure 13: Local phenomenon using the new custom nodalization (azimuthal sub-division) with ATHLET-CD

In JRC, the work was already finished for this task and reported in the last yearly report.

LEI, finished the ASTEC calculations and sensitivity studies on: oxidation parameters (zirconium oxidation physical laws), start of oxidation temperature, maximal hoop strain allowed before burst and axial extension of the cracking after clad burst as illustrated in **Erreur ! Source du renvoi introuvable.**. The BWR fuel rod model for TRANSURANUS code was set and calculations were run and compared to ASTEC results.

Table 7. Different parameters for the sensitivity analysis

Case 0	Basic	Zirconium oxidation physical law - BEST-FIT TBEG (minimum temperature to start the reaction of oxidation) – 700 K Burst parameters: EPMX 0.25; CRAC 0.50.
Case 1	CATHCART	Zirconium oxidation physical law - CATHART
Case 2	URBANIC	Zirconium oxidation physical law - URBANIC
Case 3	PRATER	Zirconium oxidation physical law - PRATER
Case 4	TBEG	TBEG (minimum temperature to start the reaction of oxidation) – 600 K
Case 5	EPMX	EPMX (maximal hoop creep allowed before burst, involving then the clad to burst immediately when fulfilled) - 0.4 (standard value according to manual)
Case 6	CRAC	CRAC (axial extension of the cracking after the clad burst) - 0.0 (standard value according to manual)

At SSTC-NRS the multistage approach of evaluation of the failed rod number for a VVER 1000 LB LOCA was finished, and results were reported in the task 3.2 final report:

- Calculation of power history of fuel rods for four cycles using the DYN3D code. Libraries of neutronic constants (XS) were calculated by the HELIOS code.
  Based on calculations using the RELAP5 code, the boundary conditions (external temperature of the fuel cladding Tout and external coolant pressure Pout during LOCA) were determined in the form of libraries for various relative power of the fuel rod Kr;fuel rod models were developed for the TRANSURANUS code, including the possibility of modeling the behavior of a VVER fuel rod in LOCA.
- A service module has been developed that provides calculations of the behavior of fuel rods during normal operation of the reactor and a LOCA for all fuel rods in the core.
- Libraries of accumulation of gaseous fission products during burnup were calculated for various types of fuel rods.
- Calculations of the number of failed fuel rods in the LOCA were performed (see **Erreur ! Source du renvoi introuvable.**) and the output of activity to the primary circuit was estimated.

The developed method for calculating the LOCA is ready for use at the SSTC NRS in the framework of studies of the consequences of the LOCA as state-of-the-art. If necessary, it can be adapted to other types of fuels and fuel cycles.

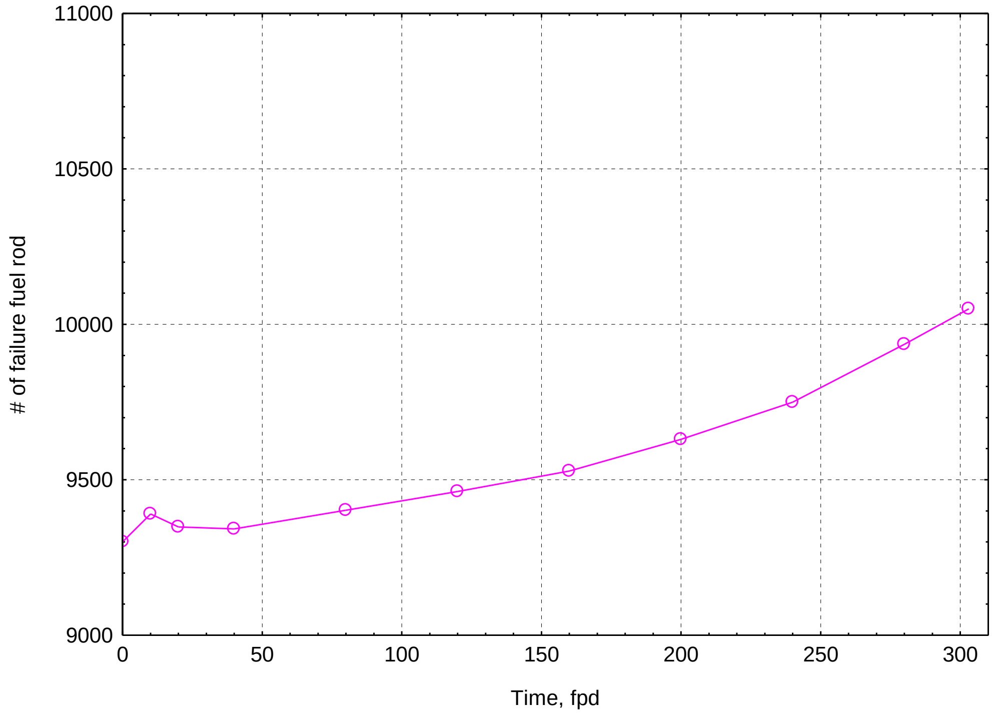

Figure 14 : Number of failure fuel rod during cycle

UJV work was already finished for this task and reported in the last yearly report. TRANSURANUS simulation of rod response to VVER-1000 LB LOCA was performed using the statistical treatment of the fuel rod and code model uncertainties combined with the sensitivity study with respect to the rod power.

The critical group of the rods with a burnup of 15 – 20 MWd/kgU was studied as only these rods have high enough power to fail during the postulated LB LOCA. The correlation between the burst time and rod power was studied as the burst time is critical to the realistic radiological consequence calculations (see. **Erreur ! Source du renvoi introuvable.**). The highest power rods were predicted soon in the transient when there is still a large mass release from the primary circuit to the containment. However, the cores with such high-power rods are not normally operated. For the realistic assessment of the radiological consequences, the delay between the break of the primary circuit pipe and the onset of the majority of the fuel failures may be credited.

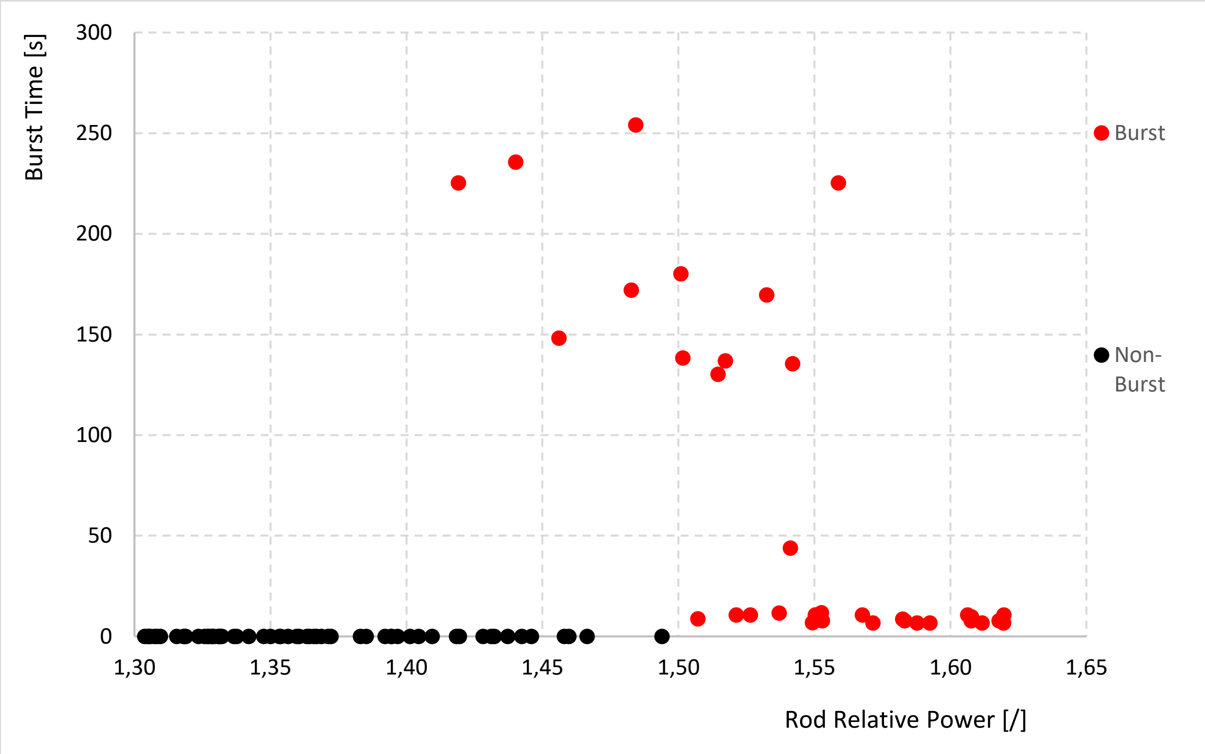

Figure 15: Rod Burst Times

VTT work carried out in this study outlines the modifications applied to the FRAPTRAN code for improved prediction of cladding behaviour during a LOCA event. Cladding deformation in BALON2 was modified by employing two high-temperature creep laws in combination with a dynamic crystallographic phase transformation model. The models are relevant for generic zircalloy and Zr1%NbO (M5) cladding types. In addition, different burst criteria were also implemented and tested. The implemented developments have been validated by detailed thermal mechanical modelling of FRAPTRAN integral assessment LOCA-tests. Furthermore, a new validation case for M5 cladding type was simulated (see **Erreur ! Source du renvoi introuvable.**). The produced results show that the original ballooning deformation dictates failure to a certain extent in most cases regardless of the burst criterion applied. Nonetheless, the newly implemented creep models are more sensitive to burst criteria as more variation is observed. [Kaddour et al, 2004] produces better predictions for M5 cladding type and more cases should be modelled with [Rosinger, 1984] creep law for accurate assessment. In terms of burst criteria, IRSN BE and IRSN max produce comparable results to the original criterion in the code. On the other hand, IRSN min and the temperature limit exhibit a more conservative boundary. Rosinger-SSM limit requires further modifications to the oxidation model before it can be used reliably. For better strain predictions, it is recommended to enable the strain limit alongside the new implemented failure criteria of temperature and stress. Further developments are suggested for improved predictions in future work:
The implemented high-temperature creep laws could be updated in terms of excess oxygen to account for embrittlement effect. Calibrated models have been published in the open literature [Jernkvist, 2021].
With respect to phase transition, creep calculations in the mixed phase region could be updated in line with latest studies in the literature and hydrogen effect should be considered for Zr1%NbO cladding types.
Additionally, [Leistikow and Schanz, 1987] oxidation model is suggested in FRAPTRAN for consistent use of Rosinger optimised limit and [Forgeron et al., 2000] limit. Since these criteria have been calibrated based on that model.

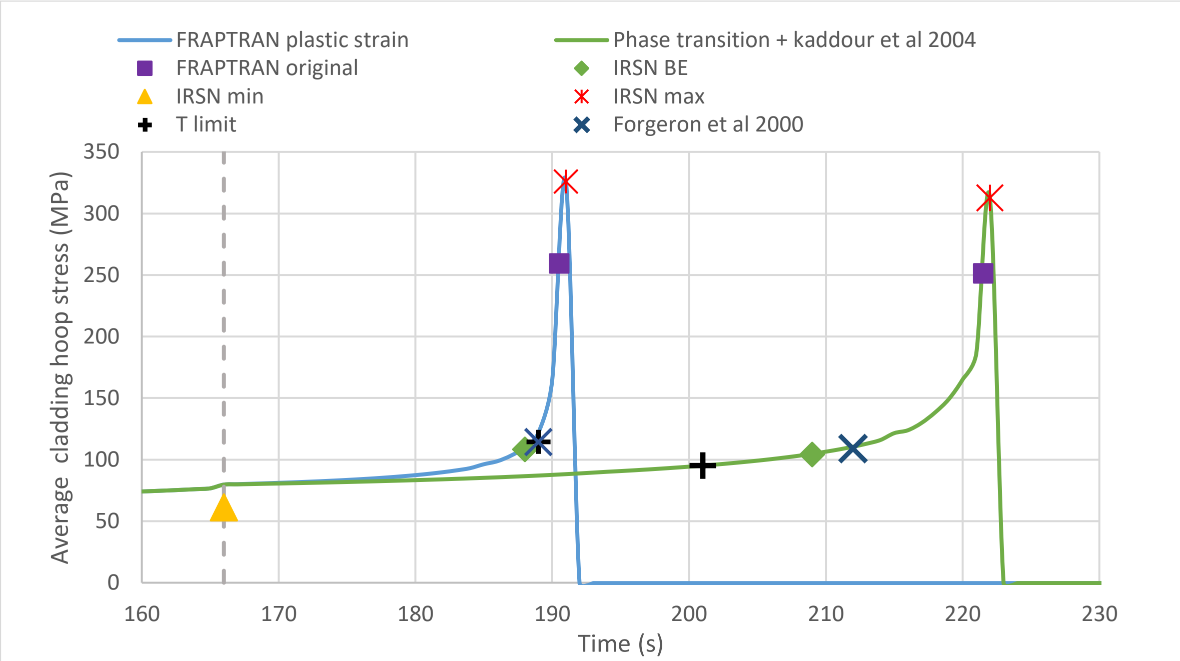

Figure 16: FRAPTRAN stress calculations with different deformation models and burst criteria for IFA-650.15

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2.3.3.3 Task 3.3: Fuel rod behaviour during LOCA

The main objective of task 3.3 was to extend the knowledge and ability of simulation codes to predict the complex fuel behaviour during a LOCA transient. Among other items, it concerns:

- The fission gas release causing additional cladding internal loading.
- The quantity and nature of radionuclide released within LOCA conditions (including rapid transients, high temperature and HBS).
- The impact of oxidation on fission gas releases.

The task has been finalized in the 3rd year of the R2CA project. As its main achievement, a higher degree of mechanistic modelling has been successfully implemented in the fuel performance codes, along with an improved viscoplastic model of the cladding.

Six organizations were involved in this task (JRC, IRSN, POLIMI, UJV, CIEMAT, SSTC and LEI), and details of the related work are covered in the final task report (project deliverable D3.6). The progress made in the last reporting period can be summarized as follows:

At CIEMAT, the integral fuel performance code FRAPTRAN has been extended in terms of mechanical modelling, more precisely by adapting an alternative Norton-type creep law and cladding failure limits – including bias options. The FRAPCON code [Geelhood, 2015] has been coupled with the SCIANTIX mesoscale model [Pizzocri, 2020]. Its evaluation is still underway in the frame of a mobility plan and is reported separately. SCIANTIX models for fission gas behaviour have been refined by increasing numerical stability and a priori error control under transient conditions.

The JRC has been working closely with IRSN and POLIMI on coupling the TRANSURANUS code with two mesoscale fuel behaviour codes (MFPR-F [Veshchunov, 2006] (**Erreur ! Source du renvoi introuvable.**) and SCIANTIX). Considerable effort has been made to develop plug-in modules that allow for: a) feedback from these codes to the integral fuel simulation, including mechanical phenomena as e.g. fuel deformation, and b) applying a re-start modification option as needed for the simulation of a LOCA following a base irradiation in a commercial NPP.

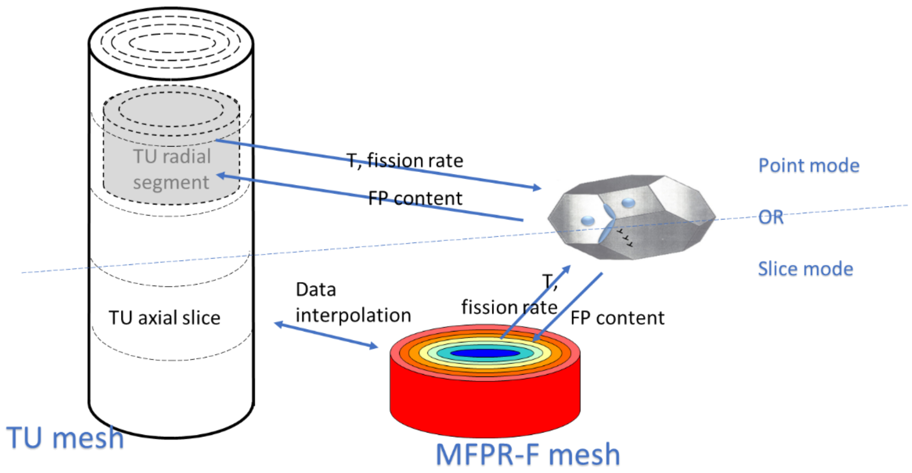

Figure 17: Scheme for the TRANSURANUS//MFPR-F coupling in point mode (top) or slice mode (bottom).

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

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

For the assessment of the modified simulation tools, a number of cases from the IFPE database [IFPE, 2018] (maintained at the OECD/NEA) has been selected. They cover two LOCA experiments of the Halden Reactor test series IFA 650, one LOCA simulation test performed by Studsvik Nuclear AB, Sweden (NRC-192), as well as 3 transient irradiation experiments at the French Siloe reactor (HATAC C1 and C2, Contact 1). The available experimental data, power histories and boundary conditions were used for verification and validation of the coupled code versions. The LOCA cases show agreement with the outcome of the IAEA FUMAC project [FUMAC, 2018], and a small impact of the various approaches for simulating fission product behaviour on cladding deformation and rupture (**Erreur ! Source du renvoi introuvable.**).

This is also consistent with the first uncertainty and sensitivity analyses for the LOCA phase of IFA 650.10 and IFA 650.11, carried out at JRC. They confirm the expected dominance of the cladding outer temperatures for calculating the deformation of the cladding up to the time of burst, and indicate the importance of cladding material properties, as creep, swelling and the elasticity module. Further analysis is however needed before setting priorities for further code development, and an additional scheme of Monte-Carlo runs with restricted input uncertainties should be set up.

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

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

All work related to the coupled modes of TRANSURANUS was performed in collaboration with JRC and presented at two international workshops "Towards nuclear fuel modelling in the various reactor types across Europe", 28-30 June 2021 (online) and 22-23 September 2023 (Bologna, embedded in the R2CA progress meeting).

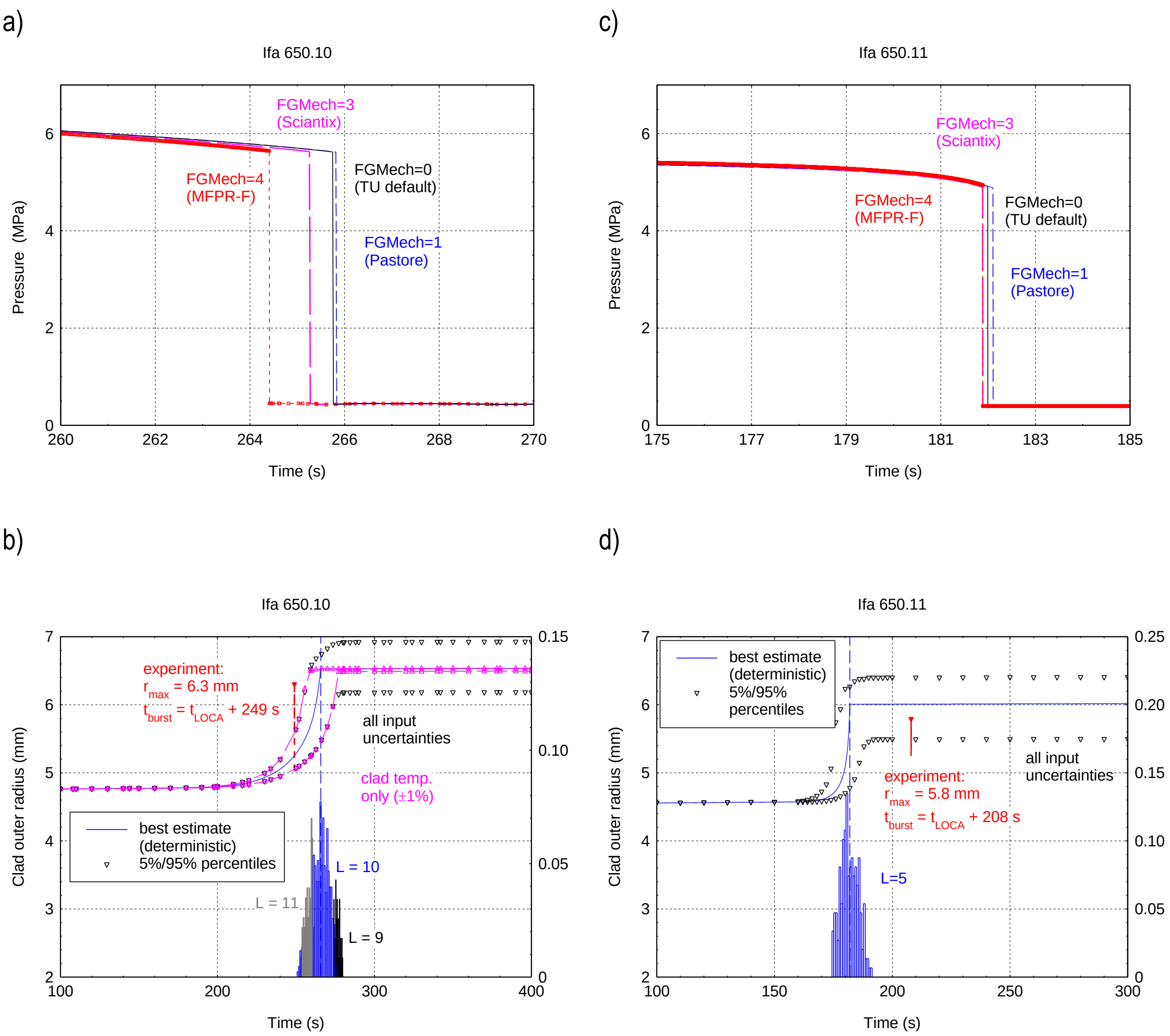

Figure 18: Inner pin pressure (a and c) and cladding outer radius (b and d - at axial location of maximum ballooning) as function of time during LOCA simulated with different options of the latest version of TRANSURANUS, for the Halden LOCA tests Ifa 650.10 and Ifa 650.11, respectively.

Finally, at CIEMAT the extended FRAPTRAN code has been verified using the IFA 650.10 LOCA test (**Erreur ! Source du renvoi introuvable.**, **Erreur ! Source du renvoi introuvable.**) and the standalone PUZRY tests (both taken from the IAEA FUMAC project). A detailed analysis of both tests confirmed that FRAPTRAN (applying either MATPRO or Norton creep laws) gives rise to conservative results of the time-to-failure. Improvements in the time-to-failure prediction are primarily linked to the visco-plastic performance of the cladding while modified failure limits will not lead to higher accuracy. A final implementation of Norton´s creep law would require the irradiation hardening effect to be included.

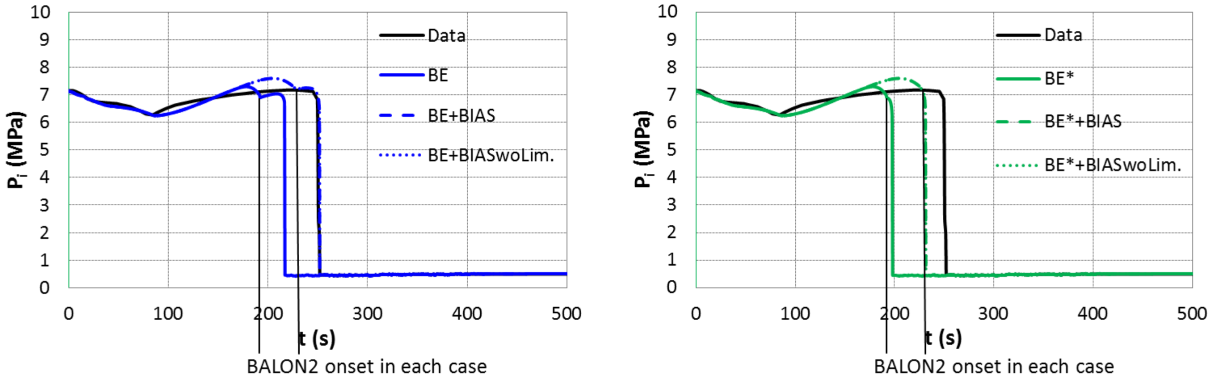

Figure 19: Model-to-data comparison for the internal pressure (P_i) in IFA-650.10. Predictions with MATPRO´s creep model on the left and with Norton´s law on the right.

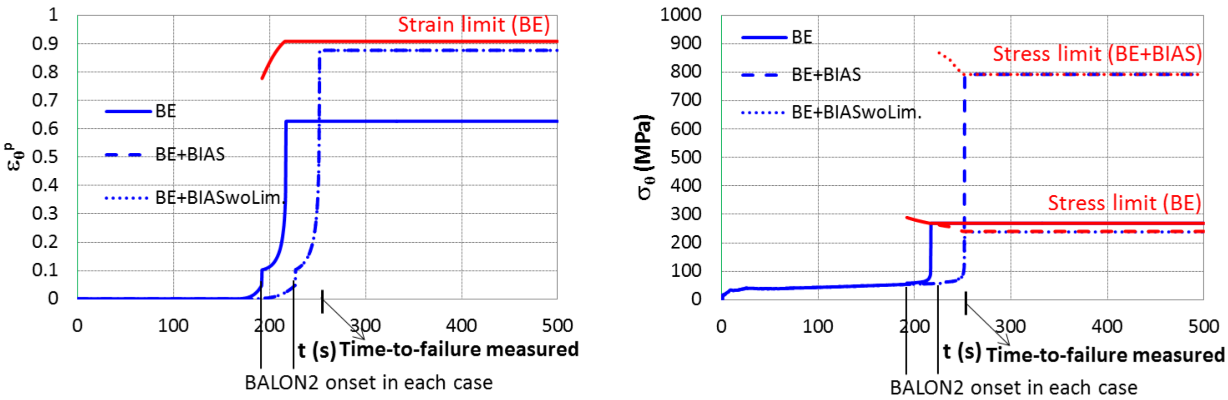

Figure 20: Predictions in IFA-650.10 with MATPRO´s creep model. Cladding plastic hoop strain on the left and hoop stress on the right.

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2.4 WP4-SGTR

2.4.1 Objectives

This Work Package aims to improve the different simulation tools and models used to analyse the SGTR transients for a better evaluate of their corresponding releases into the environment within DBA and DEC-A domains. It is focussed on the behaviour defective fuel rods in a core and on FP (focused on Iodine) behaviour in the damaged Steam Generator. To that extent, existing databases and models have been revisited.

More especially, 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 (lead by CIEMAT)
- Task 4.2: Fission product release from defective fuel rod during SGTR transient (including the iodine spiking phenomena) (lead by POLIMI)
- Task 4.3: Secondary hydriding phenomena of defective fuel rod clads in normal operation and subsequent clad failure under SGTR transients (lead by IRSN)

2.4.2 Overview of the main advances

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

- In order to improve the simulation of fission product releases during a SGTR transients, code capabilities have been reviewed and then enhanced with external functions or user's driven coefficients (MAAP, RELAP, MELCOR, ASTEC (incl. iodine peak releases into RCS, iodine transport from primary-to-secondary into the failed SG). Focus was done on the transport of radioactive iodine, but some analyses included a rather large number of other fission products, too (i.e. Cs). A special attention is also paid to partitioning and steaming phenomena in the damaged steam generator (ASTEC, MELCOR).
- New physico-based models/correlations for simulating the behaviour/release of FP (esp. gaseous and volatile FPs such as Iodine and Caesium) from fuel to gap have been developed and implemented (including FP generation/decay in fuel; FP diffusion as a function of fuel oxidation…) in TU, SCIANTIX, MFPR-F, RING codes mainly. These have been verified upon increased FP releases from fuel observed in experimental irradiation tests and NPP experimental measurements with linear heat rate changes/power transients. In addition, for simulating the gap-to-coolant releases a calibration of the gas escape coefficients has been performed, further verified upon the CRUSIFON experimental tests.
- From the experimental data of H uptake rate and total absorption in E110 (valid for 300≤T≤400°C and P_{H2}≤ 0.4 bar) two basic numerical different models was developed as already implemented models (i.e. in TRASURANUS fuel performance code) initially developed for higher temperatures were found to be not applicable wo a re-evaluation of key parameters. A multi-physical model for the overall phenomena occurring during secondary hydriding form water ingress up to hydrides blister formation was also developed in SHOWBIZ using pre-existing models for H redistribution. The results of this model were compared with the HYDCLAD model developed by CIEMAT during the 2nd project year.

2.4.3 Details of the activities performed

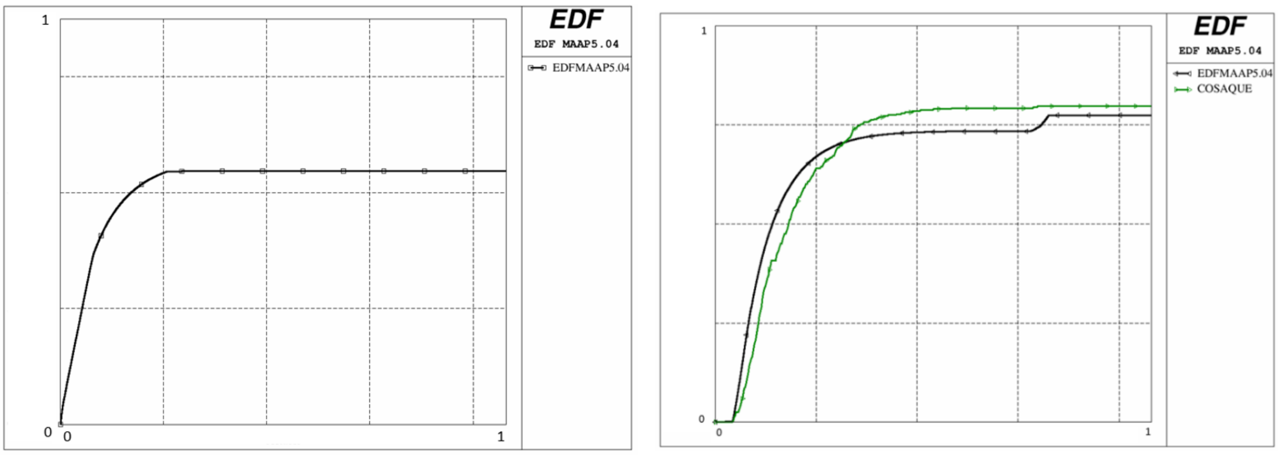
2.4.3.1 Task 4.1: Fission product transport and releases from primary circuit to environment

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 was gathered and their suitability to the conditions of interest assessed. Proposals, if necessary, for improvement/adaptation of integral computer codes have been ongoing.

The objective for this third year was to progress in the improvement/adaptation of models used in integral codes, as said above. The outcome of the work will be gathered in the planed deliverable: “Final report on experimental database reassessment and on model/code improvements for fission product releases during a SGTR transient (D4.1.2), which was supposed to be released by 31.08.2022 and it has been postponed due to delays in partner’s progress. The foreseen date for D4.1.2 is 31.03.2023.

A brief information of the work done during the third year follows.

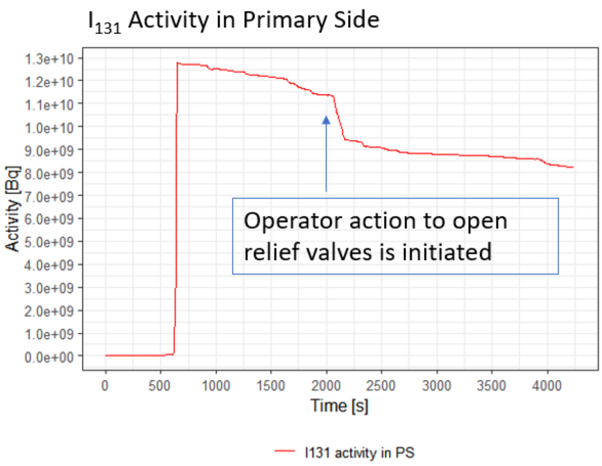
During the past year, EDF continued enhancing and verifying the models implemented in MAAP for the FP releases from the primary side to the secondary side and eventually to the environment. Some improvements have been made by considering specifics of different FP species (noble gases, iodine, caesium…) 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 testing of the enhanced MAAP performance has been carried out through comparisons to COSAQUE (EDF reference code for activity calculations) predictions on 2 different types of plants: PWR900MWe (3 loops) (**Erreur ! Source du renvoi introuvable.**) and PWR1300MWe (4 loops). Both codes showed a remarkable similarity. It is planned to extend the comparisons to SGTR transients for the N4-type plant. Eventually, the intention is to activate those models for analyses of crises situation (real crises or training exercises in EDF).



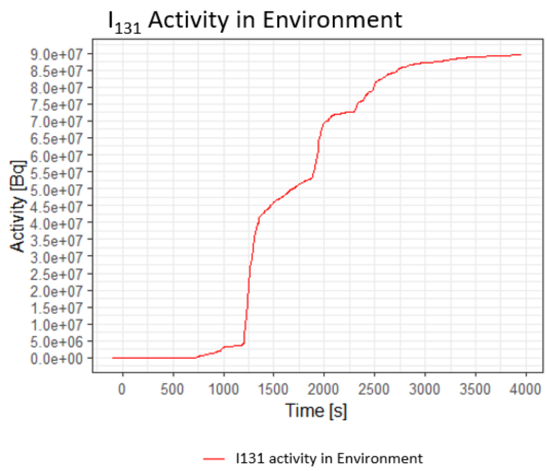
a) b)

Figure 21: SGTR initiated at full power in 3-loop PWR plant – Calculated Noble gas (a) and Iodine (b) activity released to the environment vs time with MAAP code (Verification against COSAQUE code).

BOKU has been focused on enhancing the RELAP5 capability to simulate 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 different ways of improvement are being explored. As for iodine spiking, an extensive literature survey was conducted, but few open data have been found, most of which were taken long ago. Some additional data have been found mostly referred to Western PWRs and just few to Russian VVERs. This information is being used to build an external function that feeds RELAP5 as a FP source (**Erreur ! Source du renvoi introuvable.**). BOKU's work in the upcoming months will consist of building a specific function to improve the estimate of decay chains and to develop different iodine spiking scenarios based on the empirical database gathered.



a)



b)

Figure 22: Preliminary transient calculation results of iodine activity in primary coolant (a) and environment (b) (FP transport model implemented in RELAP5-3D).

CIEMAT has selected specific valuable data from the R2CA project database concerning the FP transport. Just few data were found 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. 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 their application under the secondary side conditions of a SGTR sequence is questionable, to say the least. As a matter of fact, based on the flashing model of MELCOR a specific model for iodine primary-to-secondary transport in a failed steam generator was developed and implemented in the code using control functions.
Finally, a template for D 4.1.2 deliverable has been built and distributed to the partners.

IRSN started a vast plan for updating fission product transport in IRSN codes. The focus will be the SAFARI module in ASTEC (specifically built for SGTR accidents). Refinements needed were identified (iodine spiking; transport, deposition and transmutation of fission products; simplified nodalization; etc.). In addition, the effect of iodine speciation on its primary-secondary transfer at the breach will be studied by using the SOPHAEROS module. The intention is to transfer the results of all these studies into the SAFARI transfer coefficients. Attention will be also paid to the thermal-hydraulic phenomena prevailing at the breach, which will be explored by the DROPLET module of ASTEC.

UJV's contribution aims at stating a methodology to determine the SGTR source term (inexistant in the Czech Republic). The attempt to use ATHLET-CD for fission product transport simulation in the primary and secondary circuit was abandoned due to lack of appropriate validation experiments and NPP models. They have been working on building a standalone code using mass balance equations. Such approach will be code-independent and able to use existing and future thermal hydraulic calculations as initial and boundary conditions. Such as devised, the proposed computational tool can create standardized XML source terms, which can be used directly by codes for radiological consequences evaluation, such as JRODOS. The intention is to apply the code in the analysis of a DBA SGTR event at VVER-1000/V-320, including a sensitivity study.

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 improve predictions of the complex fuel pellet behaviour in defective rods during a steam generator tube rupture (SGTR) transient and iodine accumulation phenomenon. This includes:

- Release of gaseous and volatile fission products (FPs), particularly iodine, from defective fuel rods during an SGTR transient.
- Complex fuel behaviour in defective fuel rods (especially fuel oxidation, clad secondary hydriding).

A short overview of the work performed follows.

At UJV, TRANSURANUS code calculations were used to investigate conservative assumptions regarding the number of the failed rod in the reactor core at the initiation of the SGTR. The gap inventory of ^{135}Xe, ^{133}Xe, ^{131}I and ^{137}Cs were assessed by TRANSURANUS model for both an intact fuel rod and a fuel rod with an assumed prior cladding breach. The calculated gap inventories were compared to the coolant activities measured in a VVER-1000 plant. Several cycles with varying number of leaking fuel rods were analyzed. No clear conclusion could be made for the release rates during the normal operation, concerning small activity spikes following power changes. On the other hand, the shutdown spike activity of ^{137}Cs always corresponds to the gap inventory of the leaking rods assuming no enhanced diffusion from the fuel because of the cladding failure. This conclusion helps to justify the application of the TRANSURANUS code for the gap inventory analysis.

At POLIMI, the coupling of TRANSURANUS with SCIANTIX has been upgraded to include the restart capability, allowing more detailed simulations of validation cases: CONTACT 1 [Charles, 1983] and HATAC C2 [Faure-Geors,1990] of interest for the prediction of the gap activity in pressurized water reactor (**Erreur ! Source du renvoi introuvable.**). The ANS 5.4-2010 methodology [Turnbull, 2010] has been implemented in TRANSURANUS (JRC) and SCIANTIX [Pizzocri, 2020] (POLIMI). Moreover, POLIMI developed a methodology to bound the numerical error on the prediction of the release of radioactive gaseous and volatile fission products [Zullo, 2022a]. This methodology has been applied in the novel physics-based model for radioactive fission gas (FG) behaviour in the fuel, developed at POLIMI and implemented in SCIANTIX. The latter model has been tested in both the stand-alone SCIANTIX version [Zullo, 2022b] and the version of TRANSURANUS coupled with SCIANTIX [Zullo, 2022c], thanks to the collaboration between JRC and POLIMI. Results have been published in three journal papers [Zullo, 2022a; Zullo 2022b; Zullo 2022c].

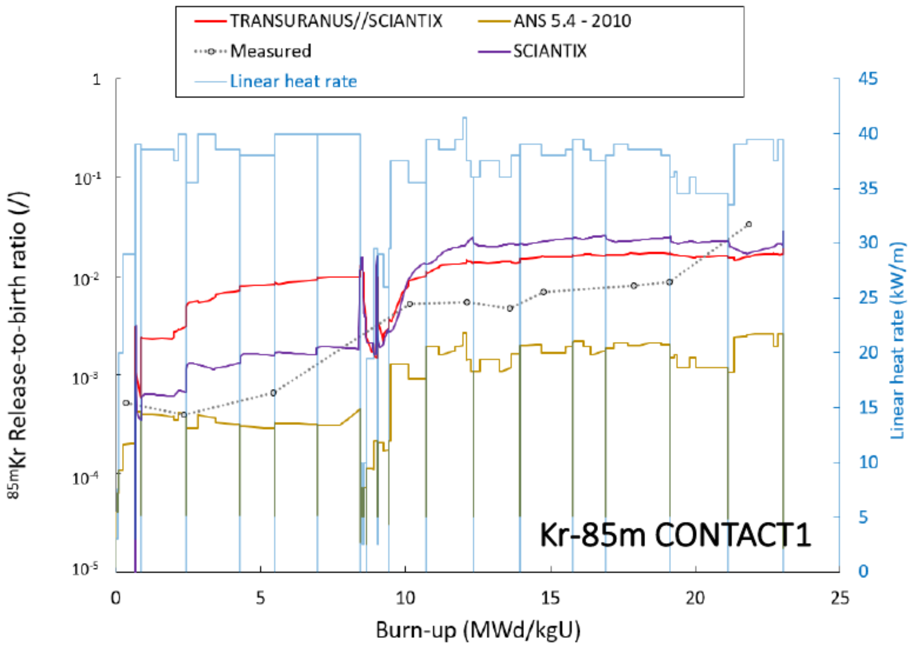
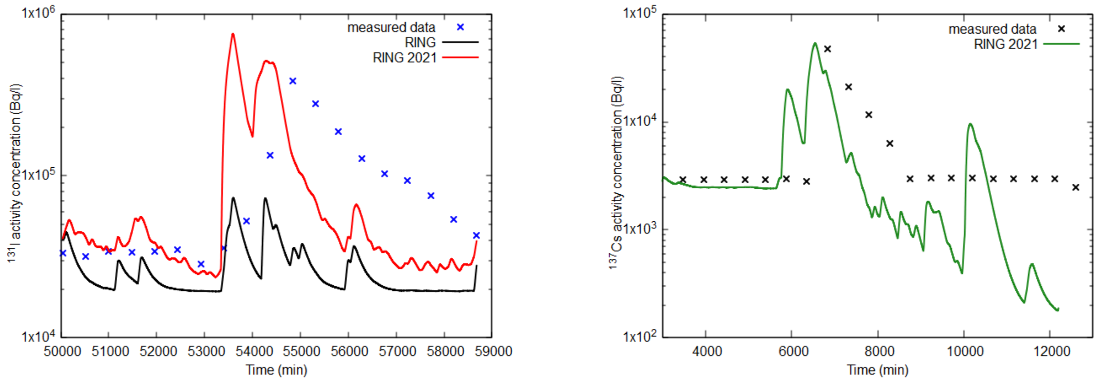


Figure 23: Release-to-birth ratio of Kr-85m during CONTACT1 experiment - Comparison between SCIANTIX calculations (stand-alone mode and coupled with TU) with experimental data

IRSN proposed a new methodology for evaluating the release of radioactive isotopes from the fuel, by treating separately the release problem of (stable) elements, and the decay/release problem of radioactive isotopes. This allows to perform accurate assessment of the element release, and then to reuse this assessment for the calculation of radioactive isotope release. This methodology, called "decoupling approach", uses two separate tools: the coupling of TRANSURANUS and MFPR-F codes, developed in collaboration with JRC, and a simple calculation tool for the formation, decay, and transmutation of radioactive isotopes. This approach is applied as an illustration to an irradiation case taken from the Halden database (IFA-650.10).

BOKU has initiated a PhD position focused on modelling iodine spiking. A review of current literature was conducted. Simulations have been performed with RELAP5-3D. For WP2 transient calculations, the FP transport model of RELAP5-3D has already been implemented. A preliminary evaluation revealed that the FP behaviour model incorporated in RELAP5-3D is not including any physical retention effect on iodine (e.g., pool scrubbing) and is not suitable for simulating the iodine spike phenomenon without any post-processing. Therefore, an external function was introduced to improve the FP behaviour.

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 iodine concentration evolution in previous version of the code (**Erreur ! Source du renvoi introuvable.**a), and the introduction of new cesium spiking models (^{134}Cs and ^{137}Cs) (**Erreur ! Source du renvoi introuvable.**b). 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.



a) b)

Figure 24: Measured and RING calculated primary coolant activity concentration evolutions of I-131 (a) and Cs-137 (b) on power change

NINE introduced in TRANSURANUS a preliminary description for fission product release from defective fuel rods. The model considers two successive steps: (1) fuel-to-gap fission product release, and (2) gap-to-coolant fission product release [Lewis, 2017]. NINE included a more detailed description of fission product production (e.g., iodine and other unstable gas has been included) through the Bateman's equations, i.e., considering decay and capture events and fission yields. The fission products production has been tested through a comparison with the neutronic code Serpent. Regarding the diffusion of isotopes in the fuel matrix, a new option has been implemented considering a correction factor related to the fuel hyper-stoichiometry [Massih, 2018]. Assessment has been carried out on the calculated release-to-birth ratio against experimental data from CONTACT1 experiment (IFPE database) (**Erreur ! Source du renvoi introuvable.**)**Erreur ! Source du renvoi introuvable.**. Moreover, a benchmark activity on the calculated release-to-birth ratio involved the TRANSURANUS version extended by NINE, the TRANSURANUS version coupled with SCIANTIX and the ANS 5.4-2010 methodology, implemented in TRANSURANUS as mentioned above, against the CONTACT1 experiment. The gap-to-coolant release of radioactive fission products from defective fuel rods required the calibration of the gap escape rate coefficients [Veshchunov, 2019]. The calibration has been done through available experimental data of the CRUSIFON1-BIS and CRUSIFON2 experiments of the IFPE database. The results of the mentioned benchmark activity on the fuel-to-gap radioactive release and the calibration of the escape rate coefficients for the gap-to-coolant have been collected for the submission to the special issue of Annals of Nuclear Energy.

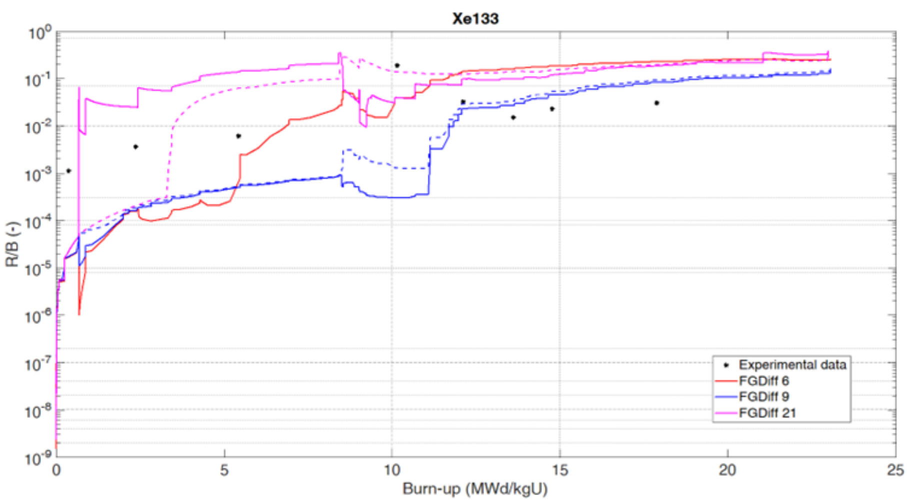


Figure 25: Release-to-birth ratio for Xe-133 during CONTACT1 experiment - Comparison between TRANSURANUS calculations including fuel oxidation with experimental data

CIEMAT has performed a critical assessment of the applicability of MELCOR FP and aerosol release models for SGTR sequences in DBA and DEC-A conditions.
Based on this, because of the limitations found for the modelling of the iodine spiking issued from the condition of fuel cladding temperature, it was decided to build an external function to model specifically the iodine behaviour during SGTR sequences. From literature review [Lewis, 1997] were considered to estimate the iodine (I^{131}) release rate from gap to coolant: 1) the enhanced-diffusional release during reactor shutdown due to iodine leaching process when coolant enters the defective rod and 2) forced-convective release driven by temperature and pressure changes.
To get the release rate to be applicable in the best estimation calculations (DEC-A scenario), a defect at the bottom end of the rod was considered and the model parameters were fitted to data collected from fifteen NPPs gathered in [Lewis, 1997].

SSTC NRS reviewed the open literature about the investigation of fission product release from fuel rods under primary to secondary leaks. Main attention was paid on investigation approaches for iodine spike-effect modelling. With this respect SSTC NRS analysed the following sources:

- 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, SSTC NRS is considering collecting data for iodine spike-effect issues for Ukrainian NPPs.

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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).

Using the results of H uptake experiments, EK created a basic numerical model to calculate the hydrogen uptake rate of E110 alloy tube segments. Using the model and the initial conditions of the original experiments, we calculated the partial pressure history during the measurements to compare it to the experimental one. This model can cover the temperature range of 300-400°C and the pressure range of 0-400 mbar using the same simple formula based both on the actual temperature and the partial pressure of the hydrogen gas. The model can also calculate the amount of the total absorbed hydrogen in the samples. The EK model works well, especially at lower temperatures (**Erreur ! Source du renvoi introuvable.**). At higher temperatures it becomes conservative by overestimating the hydrogen uptake coefficient at lower pressure values. The technical report EK-2022-437-1-3-M0 gives a description of this numerical model based on the results of the H uptake tests.

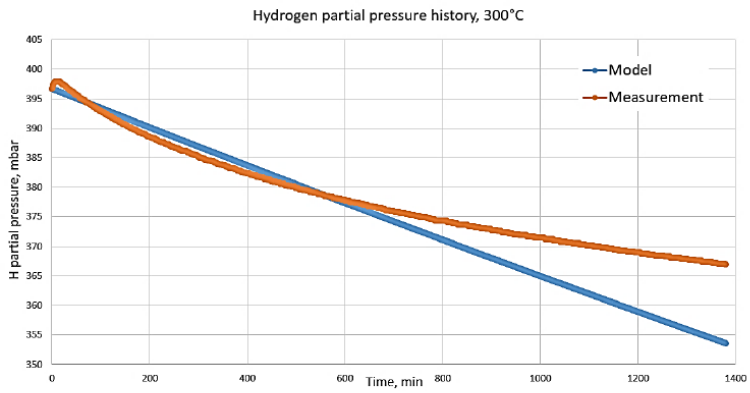
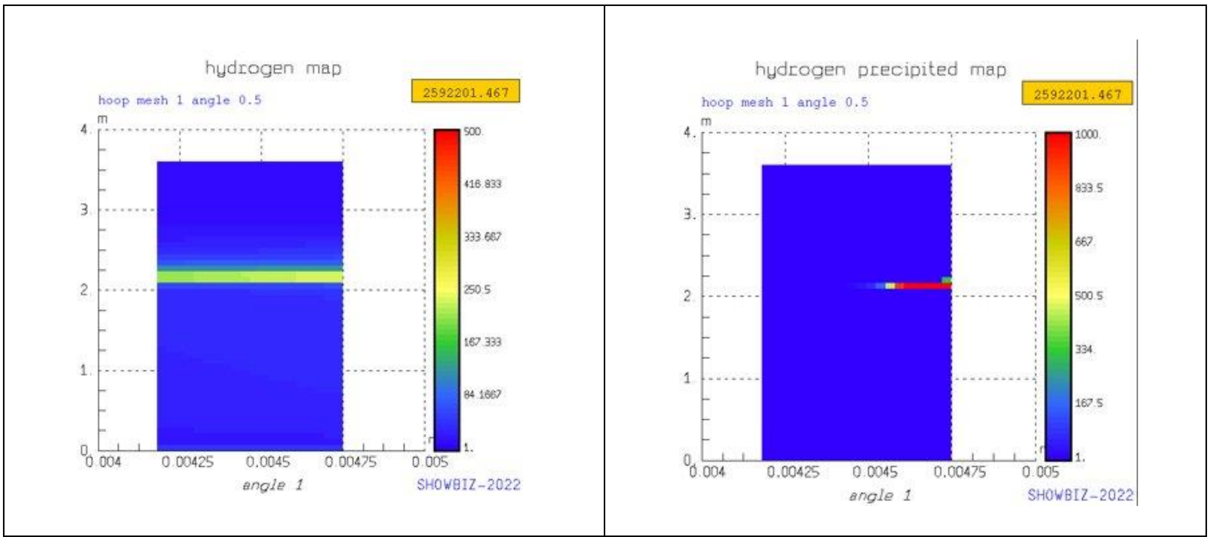


Figure 26: Comparison of the calculated pressure history and the experimental data at 300°C

IRSN has developed a multi-physics model in order to simulate the secondary hydriding phenomena from the water ingress to the formation of hydrides blister. In particular, the dedicated CHANNEL module has been implemented in the SHOWBIZ software. This module deals with the internal gas mixture and transport that are calculated together with the chemical interaction with the inner side of the fuel rod clad. A coupling of this 1D structure with the 3D cladding geometry has also been achieved and allows to consider both hydrogen and oxygen uptake coming from internal oxidation and hydriding processes. Coupling with the chemical models have also been successfully tested. Pre-existing models for hydrogen bulk diffusion were used for modelling the H redistribution in the cladding.

A massive hydriding model compatible with the SHOWBIZ software architecture has been created. It consists of a hydrogen uptake rate model determined from EK experimental data at relevant temperatures for Zircaloy-4. IRSN proposed a basic numerical model dependant on the temperature and the H_2 partial pressure. This model being different from the one developed by EK for E110.
Using representative thermal boundary condition from FRAPCON pre-irradiation reference calculation, IRSN was able to reproduce the formation of a secondary defective region with very high localized hydrogen content as a result of a water ingress in a postulated primary defect (**Erreur ! Source du renvoi introuvable.**). The IRSN SHOWBIZ software is therefore able to qualitatively model the secondary hydriding phenomena from water penetration to the formation of hydride blisters.



a) b)

Figure 27: Calculated hydrogen distribution in clad (a) and hydrides precipitation (b) with SHOWBIZ code in a defective fuel rod within normal operation conditions

The CIEMAT´s technical program dealt with the modelling of the in-clad secondary hydriding process by coupling of CIEMAT´s model with FRAPCON-4.0. A first benchmark of IRSN and CIEMAT model has been performed with boundary conditions given by SHOWBIZ calculation. Both models can reproduce the blister formation even if the redistribution of H in the cladding and thus distribution of the hydrides differs. Analysis of the results are ongoing.

The preliminary HYREDI model implemented in TRANSURANUS for hydrogen uptake under transients and radial redistribution was initially planned to be further developed in collaboration with an organisation that is not involved in the R2CA project via a bilateral agreement. However, because of the unilateral cancellation of this collaboration by that partner, and in view of the promising results obtained by Feria and co-workers in the course of the R2CA project, a new bilateral collaboration agreement between JRC and CIEMAT has been established. The objective is to implement and test the coupling of the HYDCLAD model of CIEMAT, which already accounts for the precipitation and dissolution, with the TRANSURANUS code. This coupling would be similar to that with FRAPCON. Additional financial support has been obtained from the ENEN++ project in order to boost this collaboration with a mobility grant for a PhD student from CIEMAT to JRC in Karlsruhe between February and April 2023. This will also enable the code comparison for some selected LOCA cases.

The activities of NINE for Task 4.3 included a literature study of current status about hydriding modelling in TRANSURANUS but focus on testing the TRANSURANUS model for H-uptake from NucleoCon against the data of MTA EK. The results suggest that the extrapolation of the modelling parameters in much lower temperature ranges with respect to those at which they were fitted does not allow obtaining reliable results. In the experiments of MTA EK, only the low temperature alpha phase was present, for which a re-evaluation of a key parameter seems necessary. Furthermore, the analysis also indicated that uncertainties on activation energy for H solubility should also be re-considered at such conditions, as well as the boundary conditions for the H partial pressure with respect to the total pressure to take into account the role of Ar. It should also be pointed out that neither the presence of water nor oxygen were modelled, although a thin oxide layer was observed on the sample surface, which might have inhibited or delayed the hydrogen uptake. Finally, it is suggested to analyse the model of EK mentioned above in the technical report EK-2022-437-1-3-M0.

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 near-term 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 (lead by NINE)
- Task 5.2: The development of an innovative diagnosis tool (lead by IRSN)

Task 5.3: The evaluation of Accident Tolerant fuels focussing in a first intention on the most promising and mature ones (lead by EDF).

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, from the distinctive features at the initial stage of PRISE leakage accidents in VVERs-1000 and and also taking into account the procedures prescribed in the plant emergency instructions, a concept of the accident management strategy for PRISE leakage accidents at VVERs-1000 was developed, involving the automatic identification of the considered accident based on its inherent characteristics and the automatic start-up of the algorithm for accident control. It was shown that design operation of the automatic accident control algorithm brings the reactor unit to a stable state and maintains conditionally safe conditions without any releases of FP into the environment for the entire range of possible primary to secondary leaks. Also was developed a numerical optimization method for the timing of operator actions during a SGTR for VVER 1000 and PWR. Finally, in addition, to the identification of innovative devices and management approaches based on open literature survey and from Test-Facilities to reduce the consequences of some scenarios that was reported in the previous progress report, a large study dedicated on relevant tools that can be use in the nuclear industry have shown that the best tool is the artificial intelligence for several reasons such as its capabilities to predict accurate response with the absence or limited amount of data.
- Regarding innovative diagnosis tools an innovative approach, using Artificial Neural Networks (ANN) was developed and used to make predictions for a clad defect detection. To this end, a physical model for the fission product release and activity in the primary coolant was developed to generate a computational database. This database was used to train and then test the ANN predictions both against the activity of isotopes in the coolant and against the clad defect status. 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.

Finally regarding the work on Accident Tolerant Fuels the bibliographic surveys on different concepts were completed and some extension of the fuel performance codes with various materials properties and adapted models have been performed (i.e. in TRANSURANUS, FRAPTRAN, DRACCAR). First results obtain using fuel codes customised to consider eATF properties, show that most of aATF technologies can delay the time and/or the temperature of cladding failures.

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 of the accident progression details. The idea was to transport some of these experimental facility solutions in the NPP for application to derive new approaches. That is why, during the first project period the possible applicability and advantage of test facilities instrumentation and procedures were 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.

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, analysis of the preconditions for starting of accident control has been performed and a preliminary concept of the accident management strategy in the event of a PRISE leakage accident at VVRs-1000 was developed (detailed below).
- Assessment of applicability of the developed algorithm for PRISE leak range of 10÷100 mm leaks (shown below).
- Development of a numerical optimization method for the timing of operator actions during a SGTR for VVER 1000 and PWR. The method defines targets for the accident management (i.e. reaching long term coolable conditions while keeping iodine releases to a minimum) and varies then automatically the timing of operator actions, like initiation of cool down of primary system via intact steam generators or operation of pressurizer spray system, to investigate its effect on the target parameter. The timing is then optimized numerically using a very robust (but slow) algorithm, the simplex method. The analysis is currently being performed.

As indicated earlier, at the current stage of Task 5.1, ARB's efforts have been focused on the computational justification of the AM strategy for the PRISE leak accident. This strategy is based on the results of preliminary study of the distinctive features of the initial stage of the accident and the timing for decision-making, as well as for taking management measures. Main concept of the accident management strategy for PRISE leakage accidents at VVERs-1000 was developed taking into account the above aspects and also taking into account the procedures prescribed in the plant emergency instructions. The general approach involves the automatic identification of an accident based on its inherent characteristics and the automatic start-up of the algorithm for accident control.

The automatic identification of PRISE leak accident assumes the presence of a set of certain conditions, such as an increase in absorbed dose rate (ADR) near steam lines, activation of the reactor scram due to a decrease in primary pressure or a decrease in the PRZ level under the absence of a pressure increase signal in the containment.

All accident management actions in accordance with the adopted strategy have been organized as a set of sequential actions that must be sequentially implemented within an appropriate period of time. The complete list of actions is divided into 10 separate steps 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) as shown in **Erreur ! Source du renvoi introuvable.** and listed below.

step 1. Initial actions (after start-up of the algorithm for accident control):
- ✓ Forced closing of ESG BRU-A, all SGs drain lines, BRU-SN, BRU-K (if L_{ESG} ≥3.8 m)
- ✓ PRZ heaters switching off,
- ✓ Temporary closing prohibition ESG FASIV,

step 2. Feeding of intact loop SGs with EFWPs.
step 3. Trip of MCP of emergency loop.
step 4. Forced closing of ESG FW lines (MFW & EFW).
step 5. Modification/Disabling of setpoints & interlocks to provide new modes of operation for:
- ✓ PRZ spray
- ✓ MCPs, FW, EFW, FASIVs, BRU-As of intact loops

step 6. Reduction and maintenance of primary pressure by:
- ✓ PRZ spray (from MCP discharge or Make-up), or
- ✓ PRZ SVs

step 7. FASIVs closure of intact loops.
step 8. Cooldown through BRU-As of intact loops by reduction in operation setpoints
step 9. HPIS operation monitoring/control:
- ✓ Switch off 1 (of 3) train
- ✓ Restriction on primary pressure, Maintaining dTs & L_{PRZ}

step 10. Emergency loop FASIV close

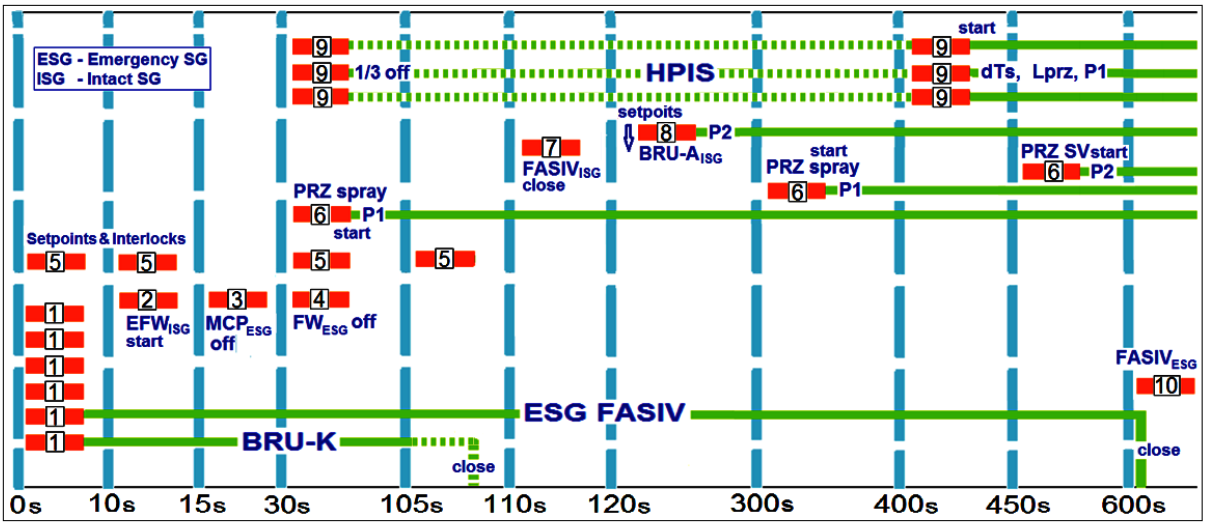


Figure 28: Algorithm for PRISE accident management in VVER-1000 (timing-actions and symptom-actions)

Design operation of the automatic accident control algorithm brings the reactor unit to a stable state and maintains conditionally safe conditions without any releases of FP into the environment for the entire range of possible primary to secondary leaks up to 100 mm in diameter. The primary pressure is maintained at a range lower than the ESG steam dump valves setpoints (**Erreur ! Source du renvoi introuvable.**) and sufficient margin before boiling in primary is provided (**Erreur ! Source du renvoi introuvable.**).

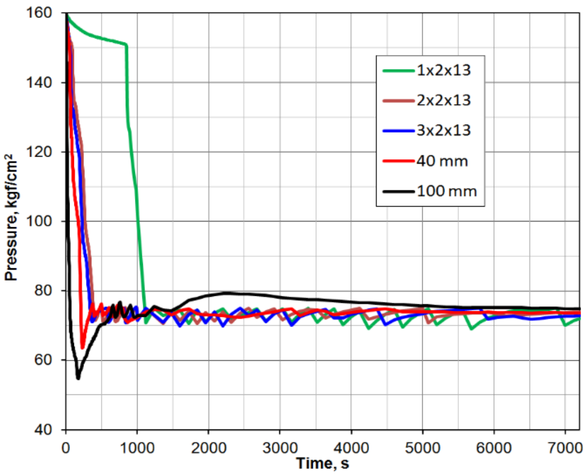


Figure 29: Primary pressure evolution during PRISE in VVER-1000 with the automatic accident control algorithm

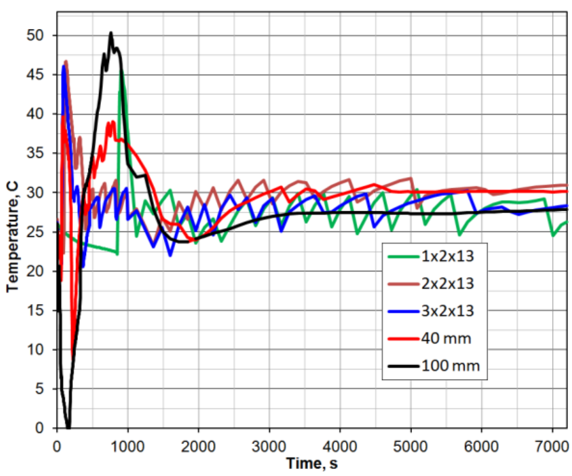


Figure 30: Evolution of the margin before boiling in primary (dTs) during PRISE in VVER-1000 with the automatic accident control algorithm

The failure of individual equipment used for accident control does not lead to a failure in accident management due to duplication of the main control functions.

In the case of a DBA or DEC-A accident scenario with non-closing of the ESG steam dump valves, the actions of the automatic management algorithm remain relevant, but appropriate and timely personnel actions are required to overcome the consequences of such an accident progression.

Meanwhile, together with the innovative strategies and instrumentation discussed so far the investigation concerned the use of tools developed for other technological areas are also considered. The investigations gave these preliminary results listed here after. Note that the listed tools are in order of possible next applicability. In addition, the listed tools are all focused on the management of the plant during an accident (but not only accident) in an autonomous way with a very limited or without the intervention of the plant operators (in a very similar way as done, as an example, for the autonomous driving of the vehicles).

Neural networks: this tool constitutes a possible substituted of the software of the system code used for simulation. In principle this tool is capable to learn and to develop its capability during time and with the availability of data to be included in its data base. It is in principle a fast-computing tool (no equations solution) and it can be very accurate. The main withdraws are constituted by the necessity to initially and properly train the net, that in simple words means to develop the necessary connections between the data; the “physic” of the phenomena is lost (or better completely implicit, the phenomenon is indirectly “hidden” in the proper connections between the data); the tool is capable to perform predictions only if data related to a specific scenario are included in its database (as a consequence a periodic updating – in terms of data and trying – is necessary to enlarge the tool capability). The tool does not have capability of prediction if data are not preventively included in the data base.

Large Data Base: this tool is very similar to the neural network. However, some differences exist. The availability of large data base in this case makes possible to associate to a combination of initial conditions and events the most resulting consequences in the data base. It works in this way: the data base collects all the available calculations and the related initial conditions, occurring events and consequences. When some initial consequences and imposed events are considered, the tool selects the consequences as the most represented consequences in the data base for those initial conditions and imposed events. Possibly percentage for different consequences could also supplied. Also in this case, a very large amount of data is necessary and the simulation of the occurring phenomena is lost. This approach is currently adopted in other technological areas (e.g. Google Translator works in this way). The tool does not have capability of prediction if specific data are not preventively included in the data base.

Artificial Intelligence: the tool uses, as the two above tools, data base. In addition, this tool includes a relevant differentiation, because it has the capability of prediction also with the absence or limited amount of data. The tool includes algorithms to perform analysis and prediction also including possibility of modification and development of suitable internal algorithms. The tool offers the capability of prediction in all the case.

A relevant aspect of this kind of tools is constituted by the acceptability of these tools not only from the technological point of view, but also from the point of view of psychological and sociological point of view for both the operators and population. However, this kind of aspects are in common to the other technological areas where those tools are in the phase of introduction (e.g., again, for example, in the autonomous driving of the vehicles).

2.5.3.2 Task 5.2: Innovative diagnosis tools

In the framework of the Task 5.2, an innovative approach, using Artificial Neural Networks (ANN), has been used to make predictions for the defect detection and characterization of fuel failures. During normal reactor operations, it is very important to detect defective fuel since continued operations under defective conditions may lead to enhanced maintenance costs for power plants. The activity of isotopes in the primary coolant is a good indicator for defect detection. As a first step in this task, a new physical model for the fission product release and coolant activity calculation was developed. Next, the physical model was used to generate the computational database for the ANN to train on. Finally, the ANN was trained on the database and then tested on a separate never-seen-before data to make predictions of coolant activity and further determine the defect status (i.e., the presence of a defect or not).

In order to develop a physical model for the fission product release and coolant activity calculation, the physical processes of FP release from a defected fuel rod need to be understood and can be categorized as a three-step process: (1) generation and transport of FP in the fuel pellet, (2) transport in the fuel-cladding gap, (3) transport in the coolant. Diffusion is considered the main mechanism for the transport of FP in the fuel matrix and, thus, a diffusion model approach (along with recoil release) was adopted for the transport in the pellet region. For the transport of FP in the fuel-to-clad gap, a generalized diffusion and first-order kinetic model was used. The transport of FP in the primary coolant was modelled using the first-order kinetic model approach.

To estimate the radioisotope activities in the primary coolant using the physical model, the mass balance equations in the three regions (Pellet, Gap, and Coolant) were solved. 8 decay chains comprising a total of 30 radioisotopes were considered. These decay chains were considered as they comprised the isotopes of interest such as noble gases (Xe, Kr) and volatile species (I). The calculations were carried out sequentially in the pellet, gap, and coolant regions. For the pellet region, the mass balance equations comprise the source from the FP generation and the loss by decay and through diffusion and recoil release. The release rate from the pellet is obtained by solving the mass balance equation for each radioisotope. The release rate from the pellet then acts as a source for the gap region. In the gap, the mass balance equations need not be solved as the release rate from the gap can be obtained directly from the expressions presented in [Veshchunov, 2019] and [Lewis, 1990]. The release rate from the gap, in addition with the tramp uranium contribution then acts as a source for the coolant region. The mass balance equations in the coolant comprise this source along with the loss by decay and escape to the CVCS. The activity of the radioisotopes in the coolant can then be calculated.

The values for the input parameters were adopted from literature. The total calculation time was set at $2.5*10^6$ s which is approximately 28.9 days. The total time was taken arbitrarily, but large enough to allow the FP activities in the coolant to reach steady-state condition. The time step for the time integration was taken as 40.0 s and the defect onset time was set at $8.64*10^5$ s, i.e., at 10 days. The R/B vs λ curves were plotted for the pellet and the gap regions and agreed well with literature. The evolution of the activities of the isotopes of interest in the primary coolant are plotted in **Erreur ! Source du renvoi introuvable.**.

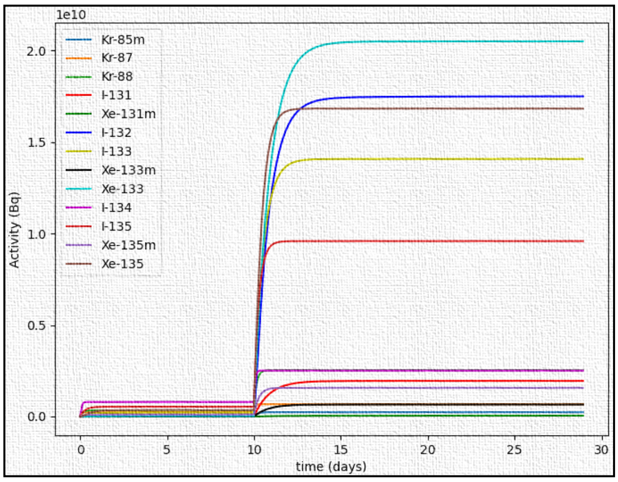


Figure 31: Evolution against time of isotope activity in the primary circuit before and after defect onset

From the analysis carried out using the physical model, it was evident that the model operates in the desired or expected manner. Apart from some neglected physical phenomena, the model produces the results which would be deemed necessary for generating the database for the ANN model.
Once the physical model was ready, it was important to have a sensitivity analysis (SA) of the model parameters to have an estimate of the best predictors (the parameters that influence the output most). Moreover, generation of the database can be done using the input parameters to get the sample file which would be used with the physical model to arrive at the different output (activity) values. In our physical model, 16 input parameters were identified which could be varied to carry out the SA as well as to generate the sample file. A single decay chain comprising 4 isotopes was considered for this analysis. The primary step for SA and to create the computational database was to generate a large sample of data. For that an in-house tool was used, comprising a collection of R scripts, to carry out the sampling of the data and for further SA. The data sampling for the possible input parameters related to the fuel pellet were done by using the TRANSURANUS code [Lassmann, 1992] in the statistics mode. For the remaining input parameters, the data was randomly sampled using the Latin hypercube sampling method. 2000 samples were generated for the 16 input parameters under the form of a comma separated value (.csv) file. Each line of the file represented one sample and was provided to the physical model to carry out the calculations of the activity. This was repeated for all the 2000 samples (lines), providing the output activity values for each calculation. The computational database for the ANN was thus generated having the 2000 samples with the 16 input parameters and the activity of the four isotopes and, separately, the defect status.

Different methods for the SA can be adopted to get the best estimates of the input parameters that impact the output the most. First, the correlation between the input parameters and the output using the partial Pearson correlation coefficient (PCC) was checked. PCC allows us to have a correlation between two variables by ignoring the contributions of the other variables and is thus more precise. At least 6 out of the 16 parameters were identified that seemed to be more strongly correlated to the activity values for the different isotopes. These parameters were the linear power, the pellet center line temperature, the cladding external surface temperature, the radius of the pellet, the gap width and the time of defect onset. The other parameters showed very less correlation with the output. This analysis gave us some idea about the more significant or influential input parameters which affect the output. In other words, it allowed us to sort out what is significant and what will be modelled as noise.

Once the computational database comprising the input parameters and the corresponding coolant activities for the four isotopes was generated, an Artificial Neural Network (ANN) was used, trained on it and tested against data that was set aside for testing. The development of this ANN was done in Python using the Keras API with TensorFlow backend. First, an ANN was used to train and make predictions about the coolant activity values of the isotopes and later it was used to make predictions about the defect status.
For the coolant activity prediction, 16 input parameters as 'features' and the activity of the 4 isotopes as 'labels' (outputs) were considered. The activities at a particular instance of time (here at t = 20 days) were considered. Moreover, through the SA performed earlier and after some analysis made during the neural network development, 8 features and 4 labels for the model development were considered. The database (2000 samples) was then split into training set (80%) and test set (20%), equivalent to a training set of 1600 samples and a test set of 400 samples. The test set was kept aside for testing the neural network.

A Sequential model was used, in which the neurons are placed in layers, sequentially. An Input Layer, two Hidden Layers and an Output Layer were considered for the model. The number of neurons in the hidden layers, along with other hyper-parameters of the model, such as batch size, number of epochs, were obtained by tuning these parameters and finding the best parameters. The other model parameters were also set. Once the best parameters were known, this sequential model was created and trained on the training set. The model also did a cross-validation along with training to have a better validation throughout training. The trained model was then tested on the never-seen-before test data set. Unlike during training, only the features were provided to the neural network, and it made predictions about the activities of the four isotopes based on its training on the training set. The predicted values of the activities of the four isotopes were then compared with the labels of the test set (the real values) and displayed in Prediction vs Reality curves for the normalized values of the activities of the four isotopes (**Erreur ! Source du renvoi introuvable.**). Almost linear plots between the activity values predicted by the ANN and the real values of activities from the test data were observed with a R^2 score quite close to 1 for all the four isotopes. On the curves there are two distinct sets of data points for the activities, with a lower set of activity values representing the observations before the defect onset or onset of defect close to the time of observation (t = 20 days) and the higher set of values representing the observations after the defect onset.

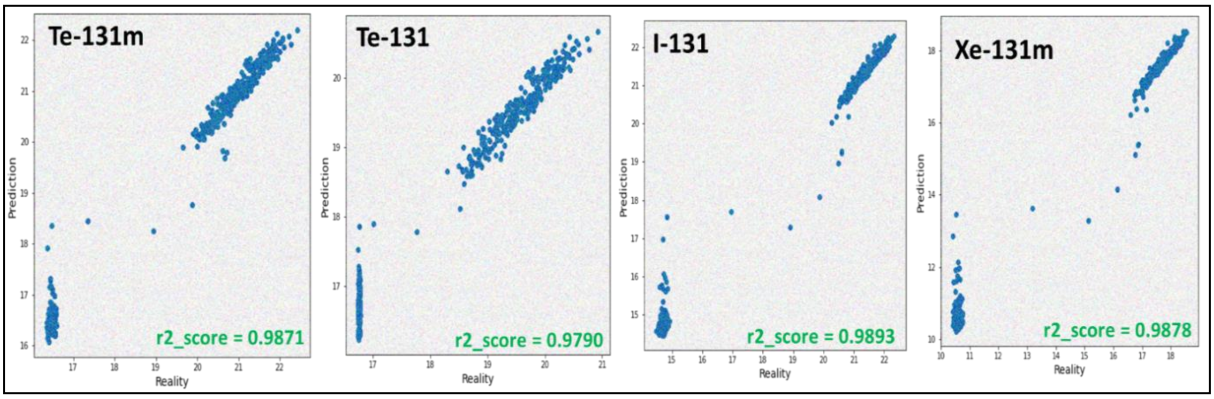


Figure 32: Prediction vs Reality curves for the normalized activity of 4 isotopes in the primary coolant

In a second step, the concept was used to make predictions about the defect status. In real case scenarios, only the isotope activity values in the primary coolant from the nuclear power plant operators are known and the objective is to predict whether there is a defect or not from them.
To have a classification whether there is a defect (1) or no defect (0), the database was modified to have the defect status as '0' for all the observations before t_defect, time of defect onset, and the defect status as '1' for all the observations after t_defect. For the defect status prediction, the activities of the four isotopes along with the linear power were used (as the linear power would be known from reactor data) as features and the defect status as the label. So, 5 features and 1 label were used for the model development. Same as before, the database was split into training and test sets. The test set is kept aside and will serve as never-seen-before data for testing the neural

network. Again, a Sequential model considering an Input Layer, two Hidden Layers and an Output Layer was adopted for the model. The hyper-parameters were tuned, and the other model parameters were also set. The tuned sequential model was trained on the training set. The trained model was then tested on the never-seen-before test data set to make predictions about the defect status. The predicted values of the defect status were then compared with the labels of the test set (the real values). Confusion Matrix was used to represent the performance of classification models like the one used here (**Erreur ! Source du renvoi introuvable.**). It uses the matrix of real and predicted values to present how accurate are the predictions made by the classification model. The confusion matrix clearly showed that the model very accurately predicted a 'defect' when there actually was a defect and 'no defect' when there actually was no defect. Only for 2 observations out of the 400 samples in the test set, the model predicted a 'no defect' when there actually was a defect. Thus, the defect status could be predicted with the artificial neural network having the coolant activities of the isotopes as input.

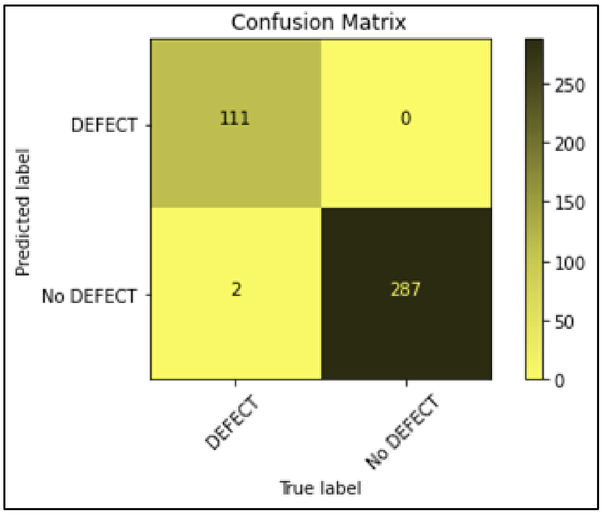


Figure 33: Confusion matrix for the defect status

To summarize, in this preliminary study, a physical model was used to generate the computational database for the ANN. Sensitivity analysis of the model parameters was carried out to have estimates of the most influential parameters. The computational database was used to train and further test the ANN to make predictions, firstly, about the activity of isotopes and then about the defect status. The ANN predicted the activity of the four isotopes with great accuracy (r^2_score > ~0.98 for each) and predicted the defect status with great precision (99.5±0.5% accuracy). The detailed results of the task have been compiled in the form of a publication which is currently under review in the journal Progress in Nuclear Energy, Elsevier Publishing [Verma, 2023].

The work carried out in Task 5.2 in the 3rd year of the project is a first step towards the development of an ANN to characterize the defective fuel rods during reactor operation. At present, the ANN deals with a classification problem, whether there is a defect or not. The objective of the ANN would be to make further predictions on the more complex defect characteristics such as the time of defect onset, the location of the defect, among others. The development in this direction is underway. Moreover, the physical model keeps updating to accommodate more physical phenomena and will be improved in the next studies. Finally, the ANN must be made time evolving as, for now, it makes predictions at a particular instance of time. These tasks are being carried out at present and will be pursued during the 4th project year.

References

K. Lassmann, "Transuranus: a fuel rod analysis code ready for use", in: Matzke, H., Schumacher, G. (Eds.), Nuclear Materials for Fission Reactors. European Materials Research Society Symposia Proceedings, 1992, pp. 295-302.

B.J. Lewis, "A generalized model for fission-product transport in the fuel-to-sheath gap of defective fuel elements", Journal of Nuclear Materials, 175, 1990, 218-226.

L. Verma, F. Kremer, K. Chevalier-Jabet, “Defective PWR fuel rods detection and characterization using an Artificial Neural Network”, Progress in Nuclear Energy, 2023 (Revision submitted).
M.S. Veshchunov, “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, 2019, pp 57-62.

2.5.3.3 Task 5.3: Advanced Technological Fuels

As already reported in the previous progress report, EDF has performed an exhaustive bibliographic review concerning the thermo-physical, mechanical behavior and the 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 main objective for the third year was with previously identified parameters and laws/material properties for the Accident Tolerant Fuels to perform simulation with fuel codes (DRACCAR, FRAPCON/FRAPTRAN, TRANSURANUS). These simulations were based on well know test case to appreciate gains that can be provided by using eATF.
In 2022, IRSN and EDF have started to model some experiments to compare in LOCA condition what are the effective gain of eATF, for chromium coating.

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.
Furthermore, as already reported in the previous report, 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 [Soti, 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 a second step, JRC implemented a first set of U_3Si_2 fuel properties in the TRANSURANUS code, which has been presented at the Pacific Basin Nuclear Conference [Van Uffelen, 2022]. Following the short overview of the implemented fuel properties, the upgraded fuel performance code was applied to a case of the FUMEX-II coordinated research project of the IAEA. The impact of U_3Si_2 fuel and FeCrAl cladding properties were first assessed on a fuel rod irradiated in a commercial nuclear power plant for which Areva provide post irradiation examination results for the code benchmark. In addition to estimating the impact of new material properties on the fuel performance, an uncertainty analysis was performed for the ATF material properties by means of the built-in Monte Carlo approach in TRANSURANUS. Analysis of the outcome by means of the TUPython tool allowed to evaluate the impact of the uncertainties of the ATF properties, and to evaluate the relative impact by means of the Pearson coefficient. The discussion of the results allowed suggesting experiments to reduce the knowledge gaps identified in the recent state-of-the-art report of the NEA.

Finally, 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 has been demonstrated that the existing FRAPTRAN model options allow to simulate the following expected behaviours of Cr-coated claddings with specific model options:

- Delayed burst.
- Lower cladding temperatures.

- Decreased ECR.

However, some code modifications in FRAPTRAN are required in order to be able to simulate the expected reduced burst strain of Cr-coated cladding. These developments will be carried out within the IAEA ATF-TS project where round robin burst tests will be performed to establish the requested creep and burst models.

Tractebel has submitted the deliverable:

- R2CA REP5.7 - Evaluation of the LOCA performance of the evolutionary Accident Tolerant Fuel (eATF) with Chromium coated Zirconium cladding with FRAPTRAN

References

Z. Soti, A. Schubert, P. Van Uffelen, "Extending the application of TRANSURANUS to coupled code calculations and statistical analyses", in: TOPFUEL 2021 (ENS, Santander, Spain, 2021).

P. Van Uffelen, A. Schubert, Z. Soti, "Assessing the effect of some ATF materials and uncertainties on their properties under normal operation conditions by means of the TRANSURANUS code", in: Pacific Basin Nuclear Conference 2022 (CNS, Chengdu, P.R. China, 2022).

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 indeed necessary to demonstrate and maximize the societal and economic impact of Project and shows the impact and benefit of European Research and Innovation fundings. The main target of the communication activity is to communicate and promote the project by informing about the project itself and its results as widely as possible. 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.

More specifically, the objectives of WP6 for the third year were to:

- Disseminate the ongoing project results (i.e. in conferences, papers in journals…)
- Perform the training on DRACCAR code
- Post the project updates and deliverables on LinkedIn and ResearchGate
- Issue the 2nd and3rd newsletters
- Complete the 2 websites
- Continue to follow the mobility program (initiating those that have not yet been launched)

Initiate a special issue for collecting papers in Open Access

2.6.2 Overview of the main advances

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

- 5 presentations in conference (NENE2022, NURETH19, ERMSAR2022, Annual Meeting of the Spanish Nuclear Society, PBNC2022)
- 2nd newsletter issued
- 3rd newsletter prepared
- All public deliverables archived in Zenodo (R2CA project community) and shared through social networks and R2CA public website
- Posts on Linkedin and ResearchGate on project updates

- 3rd annual meeting and training course on DRACCAR prepared, to be held in Bologna in September 2022
- Special issue set-up in Annals of Nuclear Energy journal by Elsevier
- R2CA website updated (https://r2ca-h2020.eu/)
- Mobilities: 1 added, 3 planned and 1 completed (over the 6 initially planned)
- PhD (1) in progress, 1 additional MSc finalized in BOKU/POLIMI, 1 post doc initiated in November 2021 in IRSN; 2 MScs to be initiated and completed during the 4th project year
- 1 training on DRACCAR /3D thermomechanical code performed by IRSN

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, **Erreur ! Source du renvoi introuvable.**, master thesis, **Erreur ! Source du renvoi introuvable.**, and training session proposals, **Erreur ! Source du renvoi introuvable.**, are available.

Along the R2CA 3rd Yearly Progress Meeting, 15 participants belonging to 7 different organizations participated to the DRACCAR software short training. This training was proposed by IRSN and hosted by ENEA in Bologna. As an introduction, the IRSN FUEL+ platform was presented to R2CA partners, it regroups a set of software focused on fuel behaviour at different scales and in different contexts – RIA, LOCA, storage & transport. Then during the training, the scope of the DRACCAR software and its specific modelling dedicated to LOCA simulation were described. In particular, the meshing allowing to represent 3D multi-rod configurations and the strong coupling between thermo-mechanic and thermohydraulic in LOCA conditions were demonstrated using simulation cases.

Table 8: Mobility proposal status

#	WP / Task	Duration	Staff involved	Envisaged period	Home organization	Host organization	Supervisor home organization	Supervisor host organization	Scientific objective	Candidate/Status
1	4.2	3 months	Post-doc/PhD	To be defined	POLIMI	JRC-Ka	Lelio Luzzi	Paul Van Uffelen	Finalize the interface between SCIANTIX and TRANSURANUS and adapt code for inclusion of the new ANS5.4 model in the code, Model benchmarking (with MFPR-F, ANS5.4, FISPRO2)	To be defined (?)
2	3.3	3 months	PhD	Sep 2022 - Dec 2022	POLIMI	CIEMAT	Davide Pizzocri	Luis E Herranz	Couple SCIANTIX with FRAPCON/FRAPTRAN for the fuel performance code to benefit from the envisaged work on fission gas behaviour modelling	Giovanni Zullo / Done
3	3.3	2 month	MSc student	Apr 2023 – May 2023	POLIMI	CIEMAT	Lelio Luzzi	Luis E Herranz	The objective of this short mobility action is to support the coupling between SCIANTIX and FRAPCON/FRAPTRAN by identifying specific developments that can be helpful from the SCIANTIX side, and the related case studies to be used for verification and validation	Giacomo Petrosillo / Planned
4	2.6	3 months	MSc student	Gen 2023 - Mar 2023	POLIMI	Bel V (Bruxelles)	Lelio Luzzi	Albert Malkhasyan	Fuel behaviour calculations with TRANSURANUS/ SCIANTIX of Belgian PWR-1000 fuel to complement CATHARE and MELCOR calculations performed by Bel V	To be defined (?)
5	3.3	2 months (in two periods)	Postdoc	30 May - 17 June 2022 22 August - 23 September 2022	LEI	IRSN	Tadas Kaliatka	Francois Kremer	Evaluation of fission product release from the high burnup structure during LOCA transient, by means of the coupled MFPR-F and TRANSURANUS codes	Andrius Tidikas / Done
6	4.1	1-2 months	PhD/Post-doc	To be defined	BOKU	NINE	Nikolaus Müllner	Marco Cherubini	Reevaluation of the fission product transport SGTR transient	Done
7	5.1	1-2 months	PhD/Post-doc	To be defined	BOKU	NINE	Nikolaus Müllner	Marco Cherubini	Optimization of accident management, evaluation of measures and benefits	Being planned

Table 9: Thesis proposal status

#	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 radioactive 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)	2021-2023	Karine Chevalier-Jabet	karine.chevalier-jabet@irsn.fr	IRSN	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	Lokesh Verma
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	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
6	4.2	9 months (MSc)	Oct 2022 – Jun 2023	Lelio Luzzi	lelio.luzzi@polimi.it	POLIMI	Implementation of a fuel oxidation model in SCIANTIX for application to defective fuel rod conditions	Giacomo Petrosillo
7	3.3	9 months (MSc)	Oct 2022 – Jun 2023	Lelio Luzzi	lelio.luzzi@polimi.it	POLIMI	Benchmark between SCIANTIX and MFPR-F capabilities for HBS formation	Edoardo Redaelli

Table 10: Training proposal status

#	Code / subject	Duration	Envisaged period	Host organization	Lecturer / Tutor	Proprietary issues	Contact	Other notes
1	TRANSURANUS / fuel performance code	1 week	January 17-21, 2022 (Karlsruhe)	JRC-Ka	P. Van Uffelen, A. Schubert, Z. Soti (JRC)	Yes	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	R2CA 1st progress meeting (On-line, October 16, 2020)	ENEA-POLIMI	D. Pizzocri and 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	2 days	19-20 September 2022	IRSN	S. Belon/T. Glantz (IRSN)	No	gaetan.guillard@irsn.fr	IRSN laptops or participant laptops if trainees have a DRACCAR user license agreement
4	TRANSURANUS+SCIANTIX / fuel performance code	1 week	June 26-30, 2023 (Karlsruhe)	JRC-Ka	P. Van Uffelen, A. Schubert, Z. Soti (JRC)	Yes	paul.van-uffelen@ec.europa.eu	Laptops of JRC are made available for trainees during course

2.6.3.2 Task 6.3: Communication and Dissemination activities

Along the third year period, the following activities have been done:

- The second newsletter has been issued (front page in **Erreur ! Source du renvoi introuvable.**)
- The third R2CA newsletter has been prepared (front page in **Erreur ! Source du renvoi introuvable.**)
- Posts on LinkedIn and ResearchGate on project updated
- Interactions initiated with the journal publisher to set up the special issue and with the partners to collect the information on the papers to be submitted
- Several scientific publications submitted:

In conferences

- Zimmerl, R., Anzengruber, L., and Mueller, N., “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”, the 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, NURETH-19, Brussels, Belgium, March 6 – 11, 2022.
- Kecek, A., “R2CA Project”, Video, 19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19), March 6–11, 2022
- Girault, N., Mascari, F., Muellner, N., Bereznhyi, A., Cherubini, M., Malkhasyan, A., Kaliatka, T., Bradt, P., Salmaoui, M., Van Uffelen, P., Arkoma, A., Hozer, Z., Jobst, M., Luzzi, L., Kecek, A., Gumenyuk, D., Pouillier, E., Herranz, L.E., “The R2CA project for evaluation of radiological consequences at design basis accidents and design extension conditions for LWRs: Motivation and first results”, the 10th European Review Meeting on Severe Accident Research (ERMSAR2022), Akademiehotel, Karlsruhe, Germany, May 16-19, 2022
- Kaliatka, T. Kacegavicius, P. and Kaliatka, A., “Analysis of LOCA Accident for BWR-4 under DEC-A conditions using ASTEC code”, the 10th European Review Meeting on Severe Accident Research (ERMSAR2022), Akademiehotel, Karlsruhe, Germany, May 16-19, 2022.
- Iglesias, R., Herranz, L.E., “Extension of the MELCOR code to DEC-A SGTR scenarios”, 47th Annual Meeting of the Spanish Nuclear Society, 28-30 September, 2022, Cartagena, Spain.
- Calabrese, R., Schubert, A., Van Uffelen, P., “Crystallographic phase transition of zirconium alloys: simulation of LOCA accidents with the TRANSURANUS code”, 31st International conference Nuclear Energy for New Euorope, NENE2022, Portoroz 12-15 September 2022.
- Kecek, A., Denk, L., “Effect of sump pH on iodine release from VVER-1000/V-320 containment during LB LOCA”, 31st International Conference Nuclear Energy for New Europe NENE2022, Bled (Slovenia) September 12 - 15, 2022

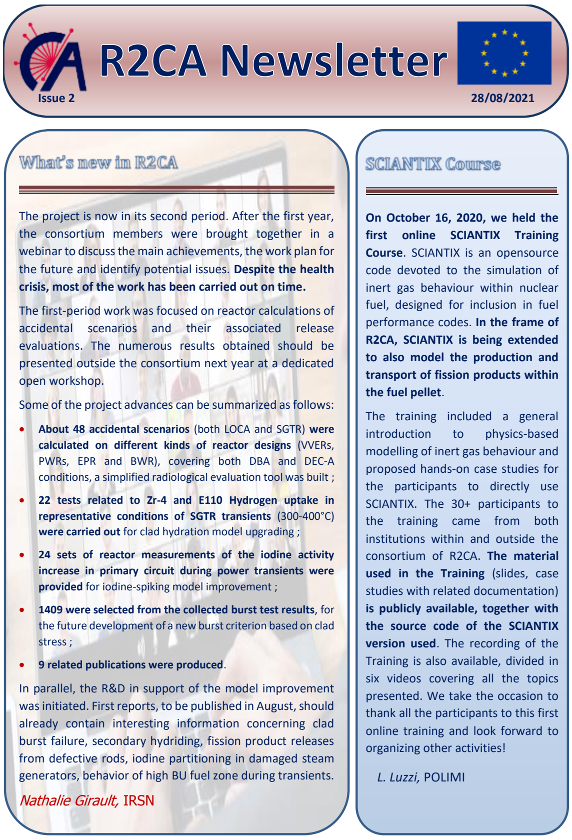
In journals

- Zullo, G., Pizzocri, D., Magni, A., Van Uffelen, P., Schubert, A., Luzzi, L., “Toards grain-scale modelling of the release of radioactive fission gas from oxide fuel: Part I: SCIANTIX”, Nuclear Engineering and Technology 54 (2022) 2271-2782
- Zullo, G., Pizzocri, D., Magni, A., Van Uffelen, P., Schubert, A., Luzzi, L., “Towards grain-scale modelling of the release of radioactive fission gas from oxide fuel. Part II: Coupling SCIANTIX with TRANSURANUS”, Nuclear Engineering and Technology 54 (2022) 4460-4473

For the time being, several R2CA-related papers were proposed for the special issue set-up in Annals of Nuclear Energy journal by Elsevier that will be submitted as they come in and published in open access. The provisional list is in **Erreur ! Source du renvoi introuvable.**.

Table 11: Provisional list of R2CA-related papers to be submitted in ANE special issue

WP	RELATED TASK		Comments
1-MANAG	–		R2CA history & project overview (editorial)
2-METHO	2.1.3	Experimental database	Review of experimental database to support Nuclear Power plants Safety Analyses in SGTR and LOCA domains
	2.3	Reactor calculations	First phase of a PWR-900 like reactor calculations (LOCA in DBA and DEC-A domains) in the frame of R2CA H2020 Euratom project
			PWR SGTR calculations within DBA conditions
			PWR SGTR calculations within DEC-A conditions
			Analytical evaluation of radionuclides release into the environment with a conservative approach to specifying the main contributors to the source term for pressurized water VVER-440&1000 type reactors
			Comparison of the results of conservative and realistic approaches to the analysis of radioactive release for LOCA of pressurized water VVER-440&1000 type reactors".
			Evaluation of radiological consequences for large LOCA accident in generic BWR-4 under DEC-A conditions
3-LOCA	3.1	FP transport & release to environment	Models improvements for FP transport & in-containment behaviour
	3.2	New burst criteria for LOCA radiological consequences assessment	Model improvements for the evaluation of failed rod number evaluation and new core modelling approach
	3.3	Fuel rod behavior	Towards more mechanistic modelling of nuclear fuel behaviour during a LOCA à voir nouveau nom "Towards simulations of fuel rod behaviour during severe accidents by coupling TRANSURANUS xith SCIANTIX and MFPR-F
		Fuel rod behavior	FRAPTRAN-2.0 modeling enhancement of clad failure of Zr-based alloys under DBA-LOCA conditions
4-SGTR	4.2	FP release from defective fuel rods	Modelling of defected fuel rods in TRANSURANUS: Assessment of fission product release from the fuel
	4,3	Secondary hydriding	Simulation of secondary hydriding in a defective fuel rod
	4.3	Secondary hydriding	Assessment of hydride precipitation modelling across fuel cladding: hydriding in non-defective and defective fuel rods
5-INNO	5.2	Innovative diagnosis tools & devices	Using a surrogate model for prediction of defective PWR fuel rods
	5.3	ATFs	Towards preliminary design calculations for application of Hastelloy cladding material



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.

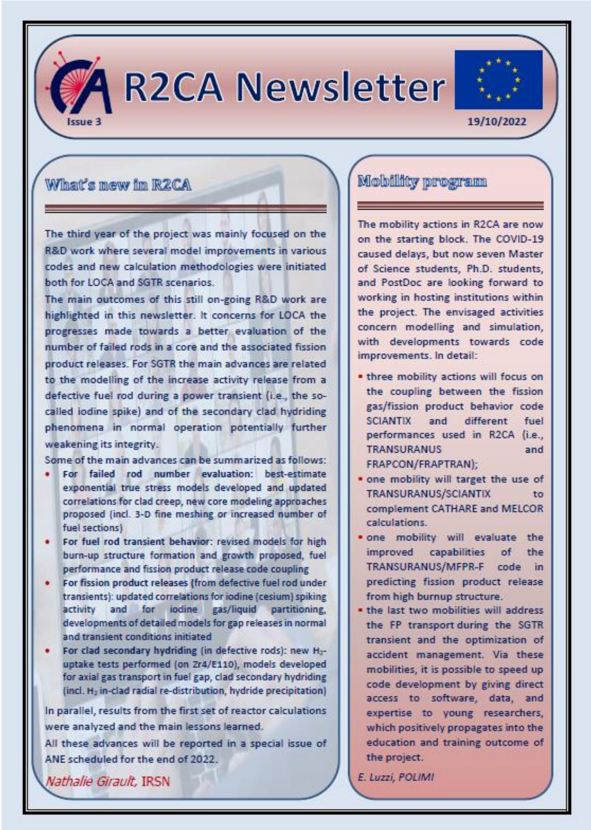
Nathalie Girault, IRSN

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



R2CA Newsletter

Issue 3 19/10/2022

What's new in R2CA

The third year of the project was mainly focused on the R&D work where several model improvements in various codes and new calculation methodologies were initiated both for LOCA and SGTR scenarios.

The main outcomes of this still on-going R&D work are highlighted in this newsletter. It concerns for LOCA the progresses made towards a better evaluation of the number of failed rods in a core and the associated fission product releases. For SGTR the main advances are related to the modelling of the increase activity release from a defective fuel rod during a power transient (i.e., the so-called iodine spike) and of the secondary clad hydriding phenomena in normal operation potentially further weakening its integrity.

Some of the main advances can be summarized as follows:

- **For failed rod number evaluation:** best-estimate exponential true stress models developed and updated correlations for clad creep, new core modeling approaches proposed (incl. 3-D fine meshing or increased number of fuel sections)
- **For fuel rod transient behavior:** revised models for high burn-up structure formation and growth proposed, fuel performance and fission product release code coupling
- **For fission product releases** (from defective fuel rod under transients): updated correlations for iodine (cesium) spiking activity and for iodine gas/liquid partitioning, developments of detailed models for gap releases in normal and transient conditions initiated
- **For clad secondary hydriding** (in defective rods): new H_2-uptake tests performed (on Zr4/E110), models developed for axial gas transport in fuel gap, clad secondary hydriding (incl. H_2 in-clad radial re-distribution, hydride precipitation)

In parallel, results from the first set of reactor calculations were analyzed and the main lessons learned.

All these advances will be reported in a special issue of ANE scheduled for the end of 2022.

Nathalie Girault, IRSN

Mobility program

The mobility actions in R2CA are now on the starting block. The COVID-19 caused delays, but now seven Master of Science students, Ph.D. students, and PostDoc are looking forward to working in hosting institutions within the project. The envisaged activities concern modelling and simulation, with developments towards code improvements. In detail:

- three mobility actions will focus on the coupling between the fission gas/fission product behavior code SCIANTIX and different fuel performances used in R2CA (i.e., TRANSURANUS and FRAPCON/FRAPTRAN);
- one mobility will target the use of TRANSURANUS/SCIANTIX to complement CATHARE and MELCOR calculations.
- one mobility will evaluate the improved capabilities of the TRANSURANUS/MFPR-F code in predicting fission product release from high burnup structure.
- the last two mobilities will address the FP transport during the SGTR transient and the optimization of accident management. Via these mobilities, it is possible to speed up code development by giving direct access to software, data, and expertise to young researchers, which positively propagates into the education and training outcome of the project.

E. Luzzi, POLIMI

Figure 34: Front page of the 2nd and 3rd 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 third year of the project covering the period September 2021-August 2022. This period was still marked by the health crisis and marked by the initiation of the war in Ukraine which impacted our Ukrainian partners in the project. This period still led to no face-to-face interactions with consortium members and has forced us to organize almost every meeting remotely. 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 (through conferences). Due to these highly disadvantageous conditions for the management and the cohesion of the whole group as well as due to some technical and scientific issues, the whole work has been delayed by several months. This concerns the reactor calculations as well as the R&D work in WP3-LOCA & WP4-SGTR.

Main advances during the third year concerns the work package dedicated to reactor calculations (WP2-METHO) and the work packages dedicated to the improvements of the modelling of the phenomena occurring during LOCA & SGTR sequences (i.e. WP3-LOCA & WP4-SGTR). Regarding reactor calculations, during this period the final report of T2.3 gathering the main outcomes of the first set of reactor calculations was issued. It included the final analysis and the main outcomes of the 48 scenarios that have been calculated covering LOCA and SGTR accidental scenarios, DBA and DEC-A conditions and 8 different reactor concepts including VVERs, PWRs, EPR and BWR-4. Corresponding excel data sheets gathering the main results (Thermal-hydraulics, thermo-mechanics, FP release kinetics…) were also completed that will feed the corresponding database. Meanwhile the second set of reactor calculations using the upgraded calculation chains (benefiting from WP3 & WP4 work) as well as updated evaluation methodologies for the activity releases into environment was also initiated.

With regard to the work packages dedicated to the improvements of the modelling of the phenomena occurring during LOCA & SGTR sequences (i.e. WP3-LOCA & WP4-SGTR), several code capabilities were enhanced either by new physico-based models, or external functions or user's driven coefficients. For LOCA conditions, it covered Zr-based alloy clad burst, clad high-temperature creep, clad crystallographic phase transition. In parallel, the coupling of fuel performance code with mesoscale tools allowed to obtain a higher degree of mechanistic modelling for the fission gases and fission product behaviour in the fuel and better estimate their releases. For SGTR conditions, the code capability enhancement covered the iodine and caesium peak release from fuel to gap-primary coolant following the power transients and iodine transport from primary-to-secondary in the failed SG such as partitioning, steaming phenomena. Additionally, regarding the risk of potential secondary inner clad hydriding and the formation of through-clad defect, models were also developed for simulating all the phenomena occurring from the defect formation from water ingress and H_2 uptake at low temperature up to the hydride blister formation in the clad. Significant progress has been made both in the development or adaptation of models and in the implementation of new chains/methodologies of calculations that should benefit the whole consortium. They were made at the cost of a certain delay of some actions which have delayed the completion of the final deliverables of each task of these WPs of about 6 months and thus have also postponed the closing of the second project period.

In WP5 dedicated to innovation, an innovative approach using Artificial Neural Network was developed to make predictions for clad defect detection. To this end, a new physical model for the fission product release and coolant activity calculation was developed to generate a computational database on which the ANN was further tested both against the activity of isotopes of interest in coolant and against the defect status. A numerical optimization method for the timing of operator actions during a SGTR for VVER 1000 and PWR has been developed as well as a specific accident management strategy for PRISE in VVERs including the the automatic identification of the considered accident based on its inherent characteristics and the automatic start-up of the algorithm for accident control. Finally, regarding evaluation of Accident Tolerant Fuels, the bibliographic surveys on different concepts were completed and some extension of the fuel performance codes with various materials properties and adapted models have been performed (i.e. in TRANSURANUS, FRAPTRAN, DRACCAR). First results with the modified fuel codes show that most of ATF technologies can delay the time and/or the temperature of cladding failures.

Communication and dissemination activities has been pursued and the first mobilities that have been delayed due to COVID 19 issues were initiated. Communication of the project results have been made through several conferences or journal papers. Finally, a special issue on R2CA gathering open-access papers was also initiated.

In conclusion, though most of the actions were delayed by several months no scientific and technical obstacles have been identified and all the actions, even if delayed, should be carried out. However, the delays in the R&D work have also led to a delay of more than 6 months in the final upgraded reactor calculations. In this perspective, the final synthesis work of the project and in particular the analysis of the improved reactor calculations and the harmonization of the methodologies for radiological consequence evaluations of LOCA and SGTR accidental scenarios within DBA and DEC-A conditions will not be able to be done within the given project time frame. An amendment for an extension of 4 months of the project (i.e. until the end of 2023) has therefore been submitted to the Commission.