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Author(s)	Asko Arkoma (VTT), Marton Szogradi (VTT), Joona Leskinen (VTT), Vincent Busser (IRSN), Francois Kremer (IRSN), Francois Jacq (IRSN), Sebastien Belon (IRSN), Martina Adorni (BEL V), Fulvio Mascari (ENEA), Stefano Ederli (ENEA), Dmytro Gumenyuk (SSTC-NRS), Oleg Zhabin (SSTC-NRS), Iurii Ovdiienko (SSTC-NRS), Ruslan Lishchuk (ARB), Stanislav Sholomitsky (ARB), Nikolaus Müllner (BOKU), Katalin Kulacsy (EK), Zoltán Hózer (EK), Adam Kecek (UJV), Matthias Jobst (HZDR), Luis E. Herranz (CIEMAT), Francisco Feria (CIEMAT), Rafael Iglesias (CIEMAT), Tadas Kaliatka (LEI), Paul Van-Uffelen (JRC), Paul Bradt (TRACTEBEL)
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Contents

Abbreviations

ANS	American Nuclear Society
ASTEC	Accident Source Term Evaluation Code
CATHARE	Code for Analysis of Thermal Hydraulics during Accident of Reactor and safety Evaluation
CCFL	Countercurrent Flow Limitation
CFX	Ansys CFX, computational fluid dynamics (CFD) software
CHF	Critical Heat Flux
COCOSYS	COntainment COde SYStem
DBA	Design Basis Accident
DEC	Design Extension Condition
ECC	Emergency Core Cooling
FGR	Fission Gas Release
FP	Fission Product
FUROM	FUel ROd Model
GENFLO	GENeral FLOw, thermal hydraulics code
GRS	Gesellschaft für Reaktorsicherheit
INL	Idaho National Laboratory
JVC	Jet Vortex Condenser
LOCA	Loss-Of-Coolant Accident
LOFT	Loss-of-Fluid Test Facility
MFPR-F	Module for Fission Product Release - France
MPI	Message Passing Interface
NPP	Nuclear Power Plant
PVM	Parallel Virtual Machine
RC	Radiological Consequences
RING	Release of Iodine and Noble Gases (code)
RPV	Reactor Pressure Vessel
SA	Severe Accident
SGTR	Steam Generator Tube Rupture
TH	Thermal Hydraulic(s)
U.S. NRC	United States Nuclear Regulatory Commission

1. Introduction

The goal of Work Package 2 of the R2CA project is to "propose harmonized methods of evaluation of the radiological consequences as a marker of safety margins of both SGTR an LOCA categories of DBA and DEC-A accidents." These methods rely heavily on dedicated computer programmes to perform assessments of radiological consequences (RC) and eventually to reduce the RC in LOCA and SGTR conditions. In the course of the R2CA project, computer codes and the methods how those codes are applied will be upgraded. Fission product release from the fuel rods in LOCA and SGTR, transport in the primary and secondary circuit, release to the containment and further into the environment are modelled. Often more than one code is needed in order to take into account the different modelling scales, resulting in calculation chains in which data is passed from one code to another. In addition, as various organizations use different codes for the simulation of one specific domain, the number of codes becomes large. Considering the above mentioned, Task 2.1.2 of the R2CA is set with the following specific goals: to understand the current status of modelling capabilities of LOCA and SGTR and to facilitate the comparison of various codes, to pinpoint the required development needs of each code, and to provide a base document that can be used later on to highlight the gains achieved by the code and methodology improvements during the project.

In Task 2.1.2, a review of simulation codes and calculations schemes for LOCA and SGTR has been performed. The report covers the capabilities of the available codes including both system codes and codes focusing on a part of the phenomenology, in particular focusing on the determination of the fuel rod failures as well as on the consequences of the failures. In connection with Task 2.1.1 (Radiological Consequences by Releases), review of the combined use of these codes in implementation of the evaluation methodologies is carried out.

Task 2.1.2 has 10 participating organizations, and the selection of codes (more than 20) covers fuel performance, sub-channel and system thermal hydraulics, radionuclides behaviour and integral system behaviour. Codes modelling only the steady-state operation have also been included (FRAPCON and FUROM) as they produce initial conditions for the transient codes and are an integral part of the calculation chain. While there exists a number of other codes for LOCA and SGTR analyses, this review focuses on the codes used in this project. The codes are listed in Table 1.1. The group of codes includes established codes that originate from the development work done for decades, as well as newer codes that have been developed just recently.

The partners involved are: VTT (task leader), IRSN, BEL V, ENEA, SSTC-NRS, ARB, BOKU, EK, UJV, and HZDR. TRACTEBEL, LEI, CIEMAT and JRC have also provided contributions to this task. As EdF is the only user of the MAAP code in R2CA, and EdF it is not taking part to Task 2.1.2, MAAP description is not included to this report.

The work of analysing and comparing various codes and the interlinkage between the codes is done as follows. First, a questionnaire chart was formulated, consisting of various models to be compared between the codes, with an emphasis on fission product behaviour. As there are codes with different modelling scales, the comparison of codes was divided into two Excel sheets: integral system codes, and fuel performance/radionuclides behaviour codes. The filled sheets are found in Section 3. Concerning JRodos, the Excel sheets were left unfilled as no other similar codes modelling the radiological consequences outside the containment are used in the project.

In Section 2, short descriptions of the codes written by the code owners or users are presented. The structure of the code descriptions in this report reflects the goals of Task 2.1.2. In addition to general overview of modelling capabilities, any possible interlinkages to other codes in the specific radiological consequences evaluation method are brought out, as well as how fission product release and transport is considered in the code, how data is passed in the calculation chain, what boundary conditions are needed, and can the code use the output of a code with more detailed modelling as its input. The relevant references are placed after each code description. Once the code descriptions were written and the Excel sheets filled, every participant of Task 2.1.2 had an opportunity to add or comment on those.

In Section 4, a summary of planned modelling improvements is given. In Section 5, summary and conclusions are presented.

Table 1.1. Simulation codes made use of in LOCA and SGTR analyses in the R2CA project.

Code	Application domain in R2CA						Applied as part of LOCA (L) and/or SGTR (S) analysis in R2CA	Code owner	Code users in R2CA
	Thermal hydraulics	Fuel performance in normal operation	Fuel performance in accidents and transients	Radionuclides in normal operation	Radionuclides in accidents and transients	Integral system code			
CATHARE	X						L & S	CEA, EDF, FRAMATOME, IRSN	Bel V, IRSN
GENFLO	X						L	VTT	VTT
RELAP5	X						L & S	INL	LEI, UJV, SSTC-NRS, TRACTEBEL
RELAP5-3D						X	S	INL	BOKU
DYN3D		X	X				L	HZDR	SSTC-NRS
FRAPCON		X					L & S	U.S.NRC	IRSN, VTT, CIEMAT
FUROM		X		X			L & S	EK	EK
SHOWBIZ		X	X					IRSN	IRSN
TRANSURANUS		X	X	X	X		L	JRC	HZDR, IRSN, SSTC-NRS, UJV, POLIMI, KIT, NINE, LEI, ENEA
DRACCAR			X				L	IRSN	ENEA, IRSN
FRAPTRAN			X				L	U.S.NRC	VTT, EK, CIEMAT
FEMAXI-6			X				L	JAEA	LEI
MFPR-F				X	X		L	IRSN	IRSN
TSKGO				X	X		S	EK	EK
RING					X		S	EK	EK
AC^2						X	L & S	GRS	ARB, HZDR
AC^2: ATHLET	X						L	GRS	ARB, HZDR, UJV
AC^2: ATHLET-CD	X		X				L	GRS	ARB, HZDR
AC^2: COCOSYS					X		L	GRS	ARB, UJV
APROS						X	L	VTT, Fortum	VTT
ASTEC						X	L	IRSN	ENEA, IRSN, LEI
MAAP						X	S	EPRI	EDF
MELCOR						X	L & S	U.S.NRC	Bel V, SSTC-NRS, UJV, TRACTEBEL, CIEMAT
JRodos					X		L	KIT	UJV

1.1 General information on LOCA and SGTR computational analyses

In LOCA analyses, fuel behaviour codes are used to assess the fuel rod dimensional changes, possible cladding burst, cladding temperature and high temperature oxidation, transient fission gas release, fuel fragmentation, relocation and dispersal. Some fuel behaviour codes calculate both the steady-state operation and transient while some codes use pre-transient data calculated with a separate steady-state code. There are a variety of levels to simulate the overall behaviour of the transient, e.g.: system codes including thermal hydraulics and reactor dynamics/physics, thermal hydraulics codes, reactor dynamics codes, and stand-alone or coupled CFD simulations. The results from these codes can be used as boundary conditions for the fuel behaviour codes. System codes may be used to calculate the containment source terms to be used as initial condition for codes calculating the radiological consequences (fission product transport and dose rates) outside the containment (such as JRodos in R2CA). Further information on LOCA analyses is provided, e.g., in the OECD state-of-the-art report on LOCA [1].

In SGTR analyses, fuel behaviour codes and/or detailed cladding behaviour codes may be used for modelling secondary hydriding phenomena of defective fuel rods and the impact on failure behaviour. Formation of secondary defects in the cladding due to hydriding could lead to increase in fuel dispersal in the primary circuit. Fuel behaviour code predictions on cladding mechanical behaviour, oxidation and hydriding can provide estimation on the cladding failure and subsequently, an estimate of the iodine source, and the production and release of other short-lived isotopes from the fuel rod to the primary circuit. Integral computer codes are used for the simulation of fission product release and transport from the core to the environment through the primary and secondary side and the containment. Particularly iodine spiking phenomena [2] and transport are of interest. Thermal hydraulic conditions during the SGTR events may be modelled with dedicated thermal hydraulics codes in order to evaluate the loading on rods during the transient.

Codes used for safety analyses should go through a verification and validation process. Validation is done against measurements from separate effect and integral experiments and/or power reactor data. A review of available data for code development and validation has been done in R2CA Task 2.1.3. Codes may have been assessed also against each other in benchmark exercises, such as in FUMAC [3]. Within R2CA, reactor test case simulations will be done in Tasks 2.3 and 2.5 that may allow some comparisons but due to country-specific presumptions permitted in the analysis, this effort will not be a dedicated benchmark exercise.

1.2 References

[1] OECD/NEA, 2019. Updated LOCA state-of-the-art report, November 2019 draft version
[2] OECD/NEA, 2014. Leaking Fuel Impacts and Practices. NEA/CSNI/R(2014)10. www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=NEA/CSNI/R(2014)10&docLanguage=En (accessed: 25 Feb. 2020)
[3] IAEA, 2019. Fuel modelling in accident conditions (FUMAC). Final report of a coordinated research project. IAEA-TECDOC-1889. www-pub.iaea.org/MTCD/Publications/PDF/TE-1889web.pdf (accessed: 25 Feb. 2020)

2. Short descriptions of the codes

2.1 CATHARE

2.1.1 General overview of the code and modelling capabilities

CATHARE (Code for Analysis of Thermal Hydraulics during Accident of Reactor and safety Evaluation) [1] [2] has been developed by four partners, the French Atomic Energy Commission CEA, the safety institute IRSN, the French utility EDF and the French vendor FRAMATOME. The objectives of the code are:

- Perform safety analyses with best estimate calculations of thermal-hydraulic (TH) transients in Pressurized Water Reactors for postulated accidents or other incidents,
- Quantify the conservative margin,
- Investigate plant Operating Procedures and Action management,
- To be used as a plant analyser in a full-scope training simulator providing real time calculations.

The description of the thermal non-equilibrium inhomogeneous two-phase flow is based on a two-fluid approach using mainly algebraic constitutive relations for the modelling of interfacial coupling, wall friction, and wall heat transfer processes. An interfacial pressure difference term has been introduced, which results in an unconditionally hyperbolic system of equations. The code is based on a two-fluid six-equation model. The presence of non-condensable gases such as nitrogen, hydrogen, air, can be modelled by one to four additive transport equations. The code is able to model any kind of experimental facility or PWR (including VVER), and is usable for other reactors (fusion reactor, RBMK, BWR, research reactors).

The numerical method in the CATHARE 2 code uses a first order finite volume – finite difference scheme with a staggered mesh and the donor cell principle. The time discretization varies from the fully implicit discretization used in the 0-D and 1-D modules to the semi-implicit scheme used in the 3-D modules. These methods are known for their robustness in a wide range of flow configurations. A hyperbolic equation system is used to ensure that the calculation problem is well placed. Finally, at each time step and for every type of CATHARE 2 module, one has to find the solution of a set of nonlinear equations: a full Newton-Raphson iterative method is then used.

The code is written in FORTRAN, and it is translated into a C++ version.

2.1.2 Fission product (FP) release and FP transport modelling in the code

CATHARE is a thermal hydraulics code, and thus, it does not consider FP release and transport.

2.1.3 Interlinkage to other codes in radiological consequences evaluation method

CATHARE is coupled with the DRACCAR code. In the R2CA framework, CATHARE will likely be used to calculate the TH boundary conditions for the DRACCAR code.

2.1.4 Further development needs

Development of the CATHARE code is not planned to be done in the frame of the R2CA project.

2.1.5 References

[1] Geffraye, G., Antoni, O., Farvacque, M., Kadri, D., Lavialle, G., Rameau, B., Ruby, A., 2011. CATHARE 2 V2.5_2 : A single version for various applications", Nuclear Engineering and Design, Vol. 241, pp. 4456-4463

[2] Emonot, P., Souyri, A., Gandrille, J.L., Barré, F., 2011. CATHARE-3: A new system code for thermal-hydraulics in the context of the NEPTUNE project. Nuclear Engineering and Design, Vol. 241, pp 4476-4481

2.2 GENFLO

2.2.1 General overview of the code and modelling capabilities

GENFLO (GENeral FLOw) thermal hydraulics code has been developed at VTT to be used for a wide range of applications [1]. The code has been written with the FORTRAN 77 standard. The applications have included modelling of BWR reactor vessel in re-criticality situations, VVER-440 severe accident analysis, and serving as subchannel thermal hydraulics (TH) code coupled with the fuel performance code FRAPTRAN. The TH solution principles and models in GENFLO are based on VTT's SMABRE code [2] for LOCAs. During recent years the primary application has been in the coupling [3] with FRAPTRAN [4] for LOCA simulations. FRAPTRAN-GENFLO has been validated against the Halden IFA-650 tests [5]. Initial coupling with the SCANAIR reactivity-initiated accident (RIA) fuel performance code has also been introduced more recently [6].

The applied heat transfer correlations (cf. Table 2.1) in each phase of the boiling curve have been described in detail in [1]. Many of the heat transfer correlations in GENFLO are not standard in the field, but are fitted based on typical correlations. In GENFLO, a superposition of the various heat transfer mechanisms is assumed both in pre- and post-critical heat flux (CHF) conditions. The clad-to-coolant heat transfer along the GENFLO boiling curve is described as follows. In pre-saturation, forced convection into liquid is considered. Between the saturation temperature and the critical temperature, nucleate boiling plus convection both into liquid and vapour are taken into account as separate components. Beyond the critical temperature, heat transfer into liquid and vapour are calculated separately with film boiling and convection correlations, respectively, and summed up with the radiation heat transfer into liquid. Transition boiling phase is described only during the rewetting. Film boiling phase is initiated when the cladding temperature exceeds $T_{sat} + \Delta T_L$, where the ΔT_L is the Leidenfrost temperature difference, set to be 160 °C. In addition to the clad-to-coolant heat transfer, interfacial heat transfer is taken into account in GENFLO.

For each time-step and axial segment, GENFLO calculates the coolant temperature and the clad-to-coolant heat transfer coefficients. GENFLO contains a five-equation TH model (two energy and mass equations, one momentum equation) with drift-flux phase separation. GENFLO is fast running due to a non-iterative solution of the field equations. The code is able to simulate the long-lasting reversed core flow which is possible, e.g., in large break LOCA in EPR.

Table 2.1. Heat transfer correlations in GENFLO in various heat transfer modes [1].

Heat transfer mode	Correlation
Pre-saturation	Dittus-Boelter Reynolds number is limited between 2 x 10^3 – 1.5 x 10^6, and for simplicity, Prandtl number is set equal to 1
Nucleate boiling	Simplified fitted model: $h = (2.5 \times 10^{-4}\, P + 2000)A$ P = pressure, Pa A = 1, if the void fraction is less than 0.95, otherwise A = (1-α)/0.05 where α = void fraction
Critical heat flux	Simplified fit to typical critical heat flux correlations: $\Phi_c = (1.0 \times 10^6 + \max(0.801P - 4.64 \times 10^{-8}P^2, 0.0))B$, where $B = \min(1 - 0.6\alpha, 1 - \alpha^3, (1 - qual)^2)$ qual = mass fraction of steam over the total mass of the fluid
Transition boiling	Heat flux in rewetting transition boiling phase: $\Phi = C\Phi_c \frac{\Delta T_L (T_{clad} - T_{sat})}{(\max\ (T_{clad} - T_{sat}, \Delta T_L))^2}$ ΔT_L = Leidenfrost temperature difference, °C T_{sat} = saturation temperature, °C C = constant describing the relative efficiency of the transition boiling process, with recommended range 0.05 – 10.0, and nominal value of 0.2
Film boiling	$h = 200(1 - \alpha)D$ D = constant with recommended range 0.05 – 10.0, and nominal value of 0.2
Droplet-dispersed vapour flow	Dittus-Boelter Reynolds number is limited between 2 x 10^3 – 1.5 x 10^6, and for simplicity, Prandtl number is set equal to 1
Radiation heat transfer (heat absorption into droplets)	$h = \sigma\varepsilon(1 - \alpha)E$ σ = Stefan-Boltzmann constant ε = cladding emissivity, assumed to equal 1 E = constant with recommended range 0.001 – 1.0, and nominal value of 0.1
Interfacial heat transfer	From overheated steam to liquid droplets: $h = min(x_l, 50x_g)(7500 + 0.02\rho)F$ x_l, x_g = liquid and steam mass, kg ρ = steam density, kg/m^3 F = constant with recommended range 0.001 – 1.0, and nominal value of 0.3 Also flashing and condensation are considered.

2.2.2 Fission product (FP) release and FP transport modelling in the code

Fission product behaviour is not considered in GENFLO but instead the release of fission products can be described in codes coupled with GENFLO.

2.2.3 Interlinkage to other codes in radiological consequences evaluation method

Coupling and data transfer between GENFLO and FRAPTRAN is shown in Figure 2.1. When GENFLO is coupled to a fuel performance code, it solves the TH only once during a given instant of time. GENFLO uses boundary conditions calculated with a system code, e.g., APROS [7]. The channel inlet flow is imported from the system code separately for water and steam as well as the flow from the upper plenum to the channel. Enthalpies are also given separately for liquid and steam. The system code provides the local power history used with the coupled code.

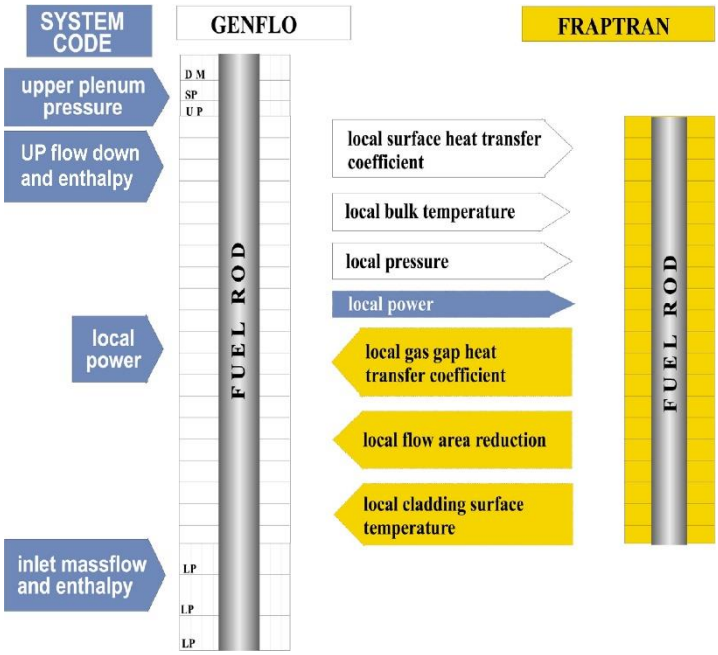

Figure 2.1. Data exchange between FRAPTRAN and GENFLO.

2.2.4 Further development needs

Coupling of GENFLO with the latest FRAPTRAN 2.0 version (released in 2016) could possibly be done within the R2CA project. The latest coupling has been established with the FRAPTRAN 1.5 version (released in 2014), and the statistical LOCA simulations [8] [9] have been conducted with the version 1.4 (released in 2011). Considerable re-writing of the code has been done between versions 1.5 and 2.0, including switching to a newer Fortran standard. Therefore, replacing the FRAPTRAN version in the coupled FRAPTRAN-GENFLO is not as straightforward as with the previous FRAPTRAN versions, and it is yet to be decided if the change is worthwhile, taking account that U.S. NRC's new FAST code is set to replace both FRAPCON and FRAPTRAN in the near future [10].

2.2.5 References

[1] Miettinen, J., Hämäläinen, A., 2002. GENFLO - A general thermal hydraulic solution for accident simulation. VTT Research notes 2163, ISBN 951-38-6083-3, ISSN 1455-0865. www.vtt.fi/inf/pdf/tiedotteet/2002/T2163.pdf (visited Feb 28, 2020)

[2] Miettinen, J., 2000. Thermohydraulic model SMABRE for light water reactor simulations. Thesis for the degree of Licentiate of Technology, Helsinki University of Technology

[3] Hämäläinen, A., Stengård, J.-O., Miettinen, J., Kyrki-Rajamäki, R., 2001. Coupled code FRAPTRAN – GENFLO for analysing fuel behaviour during PWR and BWR transients and accidents. In proceeding of: Fuel behaviour under transient and LOCA conditions, technical committee meeting, Halden, Norway, September 10-14, 2001. IAEA-TECDOC-1320

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[5] OECD/NEA, 2010. Benchmark calculations on Halden IFA-650 LOCA test results, NEA/CSNI/R6

[6] Arkoma, A., 2017. Extending the reactivity initiated accident (RIA) fuel performance code SCANAIR for boiling water reactor (BWR) applications. Nuclear Engineering and Design, Vol. 322, pp. 192–203
[7] www.apros.fi/en/ (visited Feb 28, 2020)
[8] Arkoma, A., Ikonen, T., 2016. Statistical and sensitivity analysis of failing rods in EPR LB-LOCA. In proceedings of: TopFuel 2016, Boise, Idaho, U.S.A., September 11-16, 2016, Paper 17570
[9] Arkoma, A., Hänninen, M., Rantamäki, K., Kurki, J., and Hämäläinen, A., 2015. Statistical analysis of fuel failures in large break loss-of-coolant accident (LB-LOCA) in EPR type nuclear power plant. Nuclear Engineering and Design, Vol. 285, pp. 1–14
[10] OECD/NEA, 2019. Updated LOCA state-of-the-art report, November 2019 draft version

2.3 RELAP5

2.3.1 General overview of the code and modelling capabilities

The RELAP5 code [1], [2], [3] has been developed at Idaho National Laboratory (INL) for the U.S. Nuclear Regulatory Commission (NRC) for best estimate simulation of light water reactor coolant systems during postulated transients and accidents without severe nuclear fuel damage. The RELAP5/MOD3.3 code is based on a non-homogeneous and non-equilibrium model for the two-phase system that is solved by a fast, partially implicit numerical scheme.

The modelled system is simulated by a user with a set of one-dimensional control volumes that are connected with junctions. The code provides a variety of other components (pumps, valves, pipes, accumulators, heat structures, reactor point kinetics, etc.) that can be used. Complex geometries can be represented (in simplified manner) by parallel 1-D channels that may be connected with cross-connections.

The code consists of several modules including time step control, the modules for calculating hydrodynamics, heat transfer, reactor kinetics, trips state, control variables, state of fluid in time-dependent volumes.

The thermal-hydraulic (TH) model of the code solves eight field equations (two phasic continuity, two phasic momentum and two phasic energy equations, non-condensable and boron mass conservation equations) for eight variables: pressure, phasic specific internal energies, vapour volume fraction (void fraction), phasic velocities, non-condensable quality, and boron density. The constitutive relations include models for defining flow regimes and flow-regime-related models for interphase drag and shear, the coefficient of virtual mass, wall friction, wall heat transfer, interphase heat and mass transfer, and direct (sensible) heat transfer.

Four flow regime maps are implemented in the code: a horizontal map for flow in pipes; a vertical map for flow in pipes, annuli, and bundles; a high mixing map for flow in pumps; and an ECC mixer map for flow in the horizontal pipe near the ECC injection port.

RELAP5/MOD3 uses two different models for the phasic interfacial friction force computation, the drift flux method and the drag coefficient method. The drift flux approach is used in the bubbly and slug flow regimes for vertical flow. In all other flow regimes the drag coefficient method is applied. The model uses correlations for drag coefficients and for the computation of the interfacial area density and is the model used by previous versions of RELAP5 for all flow regimes.

Several special process models are implemented in RELAP5, including abrupt area change, chocked flow, countercurrent flow limitation (CCFL), and other. A one-dimensional choked-flow model developed by Ransom and Trapp is employed in RELAP5/MOD3.3 to predict the existence of choked flow at a break or internal location and to establish the flow boundary condition if choking is predicted to occur. The model is designed to handle subcooled choked flow, two-phase choked flow (one-component and two-component), and single-phase-vapour choked flow, and can be adjusted by user-defined discharge coefficients for these conditions. Alternatively, modified Henry-Fauske model can be used to predict critical flow at system boundaries where the discharge is either into a boundary condition (time dependent volume) or into a relatively large volume simulating a containment.

CCFL option can be activated in the junctions via the user input. A general CCFL model implemented in RELAP5 allows the user to select the Wallis form, the Kutateladze form, or Bankoff weighting between the Wallis and Kutateladze CCFL forms.

RELAP5 wall heat transfer correlations are based mainly on internal flow in pipes. Additional geometries considered are vertical parallel plates, vertical and horizontal tube bundles and horizontal flat plates. A boiling curve is used in RELAP5 to govern the selection of the wall heat transfer correlations when the wall surface temperature is above the saturation temperature. The Chen boiling correlation is used up to the critical heat flux point which is predicted with a table lookup method developed by Groeneveld, Cheng, and Doan. To account the actual channel geometry, power profile and other factors the multiplying factors are used to modify the table value. The CHF-enhancing effect of the spacer grids is accounted by one of CHF multipliers (grid spacer factor) which depends on the grid pressure loss coefficient, distance to upstream spacer plane, and mass flux. The users may activate a new set of CHF correlations which were developed by the Nuclear Research Institute Rez, the Czech Republic (PG-CHF correlations).

When the wall superheat exceeds the critical value, the heat flux for both the transition boiling and the film boiling regimes are calculated with the Chen-Sundaram-Ozkaynak correlation and a modified Bromley correlation, respectively, and the maximum value is used.

For natural convection Churchill-Chu correlation is usually used for vertical geometries. If the connecting hydrodynamic volume is horizontal or when horizontal structures option is chosen (excluding the horizontal bundles), McAdams correlation is used for natural convection. For laminar forced convection an exact solution for fully developed laminar flow in a tube with a uniform wall heat flux and constant thermal properties developed by Sellars, Tribus, and Klein (Nu = 4.36) is used. The turbulent forced convection is calculated with Dittus-Boelter correlation. For vertical bundles the McAdams coefficient (0.023) in Dittus-Boelter correlation is replaced with a turbulent flow multiplier developed by Inayatov.

Condensation is calculated with the Nusselt-Shah-Coburn-Hougen correlation; and if the connecting hydrodynamic volume is horizontal, Chato-Shah-Coburn-Hougen is used.

Heat structures provided in RELAP5 permit calculation of the heat transferred across solid boundaries of hydrodynamic volumes. Heat structures are assumed to be represented by one-dimensional heat conduction in rectangular, cylindrical, or spherical geometry. Surface multipliers are used to convert the unit surface of the one-dimensional calculation to the actual surface of the heat structure. Temperature-dependent thermal conductivities and volumetric heat capacities are provided in tabular or functional form either from built-in or user-supplied data. In the reflood model a two-dimensional conduction scheme for cylindrical or rectangular heat structures is used. At the initiation of this model, each heat structure is subdivided into two axial intervals. Thereafter, the number of axial intervals is controlled by the code to efficiently use the two-dimensional conduction solution.

To define effective gas gap conductivity the dynamic gap conductance model is implemented in RELAP5 based on simplified deformation model. The model allows to account for thermal expansion of fuel pellet and cladding, radial fuel swelling and cladding creep, and cladding elastic deformation. The latter depends on a difference between coolant pressure and internal gas pressure in the gap which is calculated with ideal gas approximation. The gas composition, radial displacement values for fuel swelling and cladding creep shall be provided via user input. Material thermal expansion and elastic deformation are calculated from correspondent UO_2 and zircaloy data defined within the code.

Cladding oxidation in steam is calculated using Cathcart-Pawel correlation and the reaction heat is added to the total heat source term for the heat structure. The metal-water reaction model is coupled with the fuel rod deformation model so that if a rod ruptures, the inside of the cladding can react. The model does not account for potential steam starvation and does not alter the thermal-physical properties of the cladding as the oxide layers develop. Although the model calculates the amount of hydrogen generated, this hydrogen does not get included

into the RELAP5 hydraulic equations, nor does the steam being consumed by the metal-water reaction get withdrawn from the hydraulic equations.

To account plastic deformation of the cladding in the calculation of fuel rod's cladding temperature during LOCA simulations an empirical cladding deformation model has been incorporated into RELAP5. The model may be invoked only in conjunction with the dynamic gap conductance model.

The logical statements can be defined by user and are evaluated in RELAP5 by the trip system. The control systems typically used in hydrodynamic systems are simulated by various control system components implemented in the code, such as arithmetic, integration and differentiation control components, and others.

The power behaviour in a nuclear reactor is calculated using the point reactor kinetics model that accounts an immediate fission power and the power from decay of fission products. The user can select the decay power model based on either the American Nuclear Society (ANS) Proposed Standard ANS 5.1, Decay Energy Release Rates Following Shutdown of Uranium-Fueled Thermal Reactors, revised October 1973, or the American National Standard for Decay Heat Power in Light Water Reactors, ANSI/ANS-5.1-1979. For reactivity feedback either the separable or tabular models can be selected. In separable model each reactivity effect is assumed to be independent of other effects. The reactivity is calculated as a sum of contributors from each reactivity effect which are computed for each hydrodynamic volume and heat structure simulating the reactor core based on coolant and fuel properties in these volumes and heat structures. The tabular feedback model allows to account interactions among different feedback mechanisms and computes reactivity from multi-dimensional table lookup and linear interpolation. The average values of independent variables (e.g., coolant density, coolant temperature, fuel temperature, boron density) are obtained with the use of one weighting factor for each hydrodynamic volume contributing to reactivity feedback and one weighting factor for each heat structure contributing to reactivity feedback. Coupling of reactor kinetics with hydrodynamic and conduction/transfer calculation is explicit.

To validate the models used in the code a number of developmental assessment cases were calculated and described in [4]. These cases include: 10 phenomenological cases, which are mainly intended to demonstrate qualitatively correct functioning of the code for the relatively simple problems, as well as 13 separate effects cases and 4 integral cases, which allow qualitative and quantitative comparison of calculation results with experimental data.

The separate effect cases include Edwards pipe blowdown, Dukler air-water flooding test (CCFL), Marviken III test 24 (critical flow) and test 22 (large break flow), Loss-of-Fluid Test (LOFT) Facility accumulator blowdown test L3-1, Bennett's heated tube and ORNL bundle tests (CHF), and others (see more details in Section 2 of [4]).

The integral tests analysed as the developmental assessment cases are:

- the small break test L3-7 at the LOFT Facility: 2.54 cm break of a small pipe connected to the cold leg of a large 4-loop PWR with HPIS injection;
- large break test L2-5 at the LOFT Facility, simulating the double-ended guillotine break of the cold leg with core reflooding by hydroaccumulators, and further injection from HPIS and LPIS;
- natural circulation tests S-NC-2 and S-NC-3 in the Semiscale Mod-2A test facility (1:1705 model of the primary system of a four-loop PWR). The first of the tests simulated single-phase, two-phase and reflux natural circulation modes with a constant steam generator secondary side condition. The S-NC-3 test examined primary side two-phase natural circulation behaviour under varying steam generator secondary side mass inventory.

Based on the results of developmental assessment it was concluded that RELAP/MOD3.3 calculations demonstrate reasonable correspondence to the test results. The identified issues include [4] qualitatively incorrect results in simulations using the nearly implicit numerical option in combination with the default Henry-Fauske choked flow model, and under prediction of pressure recovery in simulation of rapid depressurization processes. However, according to Section 3 of [4] the latter issue does not appear to produce any adverse effect on the more critical safety parameter predictions such as peak cladding temperature.

Beside the developmental cases an extensive independent assessment of various RELAP/MOD3 code versions was performed in the framework of U.S.NRC Code Assessment and Maintenance Program and other research activities by various organizations applying the code. Summary of the independent code assessment reports is provided in [5].

2.3.2 Fission product (FP) release and FP transport modelling in the code

RELAP5 code does not contain mathematical models for simulation of FP release and/or transport. The user may apply available models of non-condensable gases and boron transport to obtain simplified estimates of FP transport in the primary circuit. However, this approach does not allow taking into account chemistry and phase changes, deposition and other processes of FP transport in the primary circuit.

2.3.3 Interlinkage to other codes in radiological consequences evaluation method

RELAP5 allows to estimate TH parameters of coolant being released from the primary circuit to containment in the case of LOCA or from the primary to secondary circuit and from the secondary circuit to the environment in the case of primary to secondary circuit breaks (e.g., in SGTR). The mass and energy released as a function of time can be further provided as an input to other codes that allow simulation of containment processes (e.g., COCOSYS, MELCOR). To estimate radiation consequences some assumptions (or input from other codes) need to be introduced with respect to radionuclides released. For example, for LOCA a conservative assumption on release of fuel gap activity from all of fuel assemblies or from part of FAs depending on their thermal and mechanical state can be used.

2.3.4 Further development needs

The improvement of RELAP5 by the code users to incorporate new models of fission product release, radionuclides behaviour, FP transport, etc. is not possible since the code is provided in a compiled form. Considering this, in the framework of the project the code may only be used to obtain the values of the TH parameters in the accident scenarios being evaluated. These values can further be used as an input for other codes capable of modelling the above mentioned processes.

Statistical calculation sequence between RELAP5 and TRANSURANUS (alternatively ATHLET and TRANSURANUS) will be further developed by UJV.

2.3.5 References

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2.4 RELAP5-3D

2.4.1 General overview of the code and modelling capabilities

2.4.1.1 Introduction

RELAP5-3D is a successor to RELAP5/MOD3. The code is used primarily for analysis of potential accidents and transients in water-cooled nuclear power plants, and for analysis of advanced reactor systems. RELAP5-3D provides a multi-dimensional thermal- hydraulic and kinetic modelling capability, which distinguishes the RELAP5-3D from its predecessors [1]. The multi-dimensional component in RELAP5-3D allows the user to more accurately model the multi-dimensional flow behaviour, thus removing any restrictions on the applicability of the code to the full range of postulated reactor accidents.

RELAP5-3D is a highly generic code that, in addition to the calculation of the behaviour of a reactor coolant system during a transient, can be used for the simulation of a wide variety of hydraulic and thermal transients in both nuclear and nonnuclear systems involving mixtures of steam, water, non-condensable, and solute [2, p. 33].

2.4.1.2 Software environment and code architecture

RELAP5-3D is developed and maintained at the Idaho National Laboratory (INL) for the United States Department of Energy (US DOE). The first version (1.0.0) was released in July 1997. The most recent version is 4.4.2, released in June 2018 [3].

RELAP5-3D is written in FORTRAN 95 for 32- and 64-bit computers. The fluid properties files are written in the extended Data Representation (XDR) format, while the plot files can be written in XDR or ASCII. For the code coupling capability, the coupling software is Parallel Virtual Machine (PVM) version 3.4.4. For the installation of executable code only appropriate placement of the executable on the computer platform and the availability of any required operating system libraries is necessary [4, p. 2-1].

RELAP5-3D is coded in a top-down structure with the models and procedures being isolated in separate subroutines. The top-level structure consists of:

- the input (INPUTD) block; input is processed, data input checked, and required data blocks are prepared for all program options,
- the transient/steady-state (TRNCTL) block, which handles both, the transient and the steady-state options, and
- the stripping (STRIP) block, which extracts simulation data from a plot file for further processing [4, p. 2-2]

2.4.1.3 User manuals

The code comes with a comprehensive documentation. Six user manuals are provided for a better understanding of the programme:

- Volume I: Modelling theory and associated numerical schemes [4].
- Volume II: Instructions for code application and input data preparation [5] (plus an appendix [6] providing a description of data deck organization and data card requirements
- Volume III: Results of developmental assessment cases to demonstrate and verify the models used in the code
- Volume IV: RELAP5-3D models and correlations [7].
- Volume V: Guidelines on the use of the RELAP5-3D code [8]
- Volume VI: Numerical scheme used in RELAP5-3D.

2.4.1.4 Code capabilities

The RELAP5-3D code has been developed for best-estimate transient simulation of light water reactor coolant systems during postulated accidents. The code is capable to model the linked behaviour of the reactor coolant system and the core for loss-of-coolant accidents and operational transients such as anticipated transient without

scram, loss of offsite power, loss of feedwater, and loss of flow. For the simulation of a variety of thermal hydraulic systems a generic modelling approach is used. Components of the control system and the secondary system are included to allow modelling of plant controls, turbines, condensers, and secondary feedwater systems [4, p. iii].

Relap5 is structured in components. A driver component has the task of calling the sub-components accordingly. There are three physical sub-components, the Hydro-dynamic component, the component on heat-structures, and the neutron (point) kinetics model. One component determines the state of the boundary volumes and the imposed conditions, one component determines the time step, and two components work on the logics, to model the control system of the NPP, called trips and control [2, p. 33].

The hydrodynamic model is a transient, two-fluid model for flow of a two-phase vapour/gas-liquid mixture that can contain non-condensable components and/or a solvable component [4, p. 3-1]. The thermal hydraulic system code which is used by Relap5-3D is based on the equations for mass, momentum and energy conservation of fluids to calculate the flow in the piping system. For each of the eight dependent variables a field equation is solved.

The other quantities of interest are expressed as functions of these eight variables using equations of state [2, p. 33]. For the calculation of flow regimes and flow-regime-related models for interphase friction, the coefficients of virtual mass, wall friction, wall heat transfer, interphase heat and mass transfer, and direct (sensible) heat transfer constitutive models are used [4, p. 3-161].

There are processes which are so complex in nature that Relap5-3D is modelling them with quasi-steady empirical models [4, p. 3-241]. Beside those, there are various basic models available. A Heat Structure Model for instance permits the calculation of the heat transferred across solid boundaries of hydrodynamic volumes. [4, p. 4-1]. To calculate the reactor power, either a simpler point reactor kinetics model, or a multi-dimensional neutron kinetics model based on the NESTLE code developed at North Carolina State University can be used [4, p. 7-1].

2.4.1.5 Modelling in RELAP5-3D

RELAP5-3D is capable to model multi-dimensional effects, either for fluid flow, heat transfer, or reactor kinetics. Non-detailed (one-dimensional) and detailed (multi-dimensional) simulations of fluid flow within components can be performed [5, p. 1-1].

The hydrodynamic model and the attributed numerical scheme are based on the use of fluid control volumes and junctions to display the spatial character of the flow. In Relap5-3D components are defined with a one, two, or three- dimensional array of volumes and the internal junctions connecting them. The control volumes of the one-dimensional model can be viewed as stream tubes with inlet and outlet junctions. Velocities are located at the junctions and are linked with mass and energy flow between control volumes. Control volumes are connected in series, using junctions to display a flow path. For the multi-dimensional model control volumes and junctions are also used based on Cartesian or cylindrical coordinates [5, p. 1-2].

In Relap5-3D, heat conduction flow paths are usually modelled in a one-dimensional system, using a finite difference mesh to calculate temperatures and heat flux vectors. The heat conductors can be attached to hydrodynamic volumes for the simulation of a heat flow path normal to the fluid flow path. The kinetics model consists of a system of ordinary differential equations integrated utilizing a modified Runge-Kutta technique [5, p. 1-2].

Input is characterized in terms of input records or cards, where an input record or card is an 80-character record. For legacy reasons also, input files are often referred to as decks, as in a deck of computer cards [6, p. A1-1]. For input examples see the RELAP5-3D© Code Manual Volume II – Appendix A [6].

2.4.2 Fission product (FP) release and FP transport modelling in the code

2.4.2.1 Fission product (FP) release

RELAP5-3D does not calculate fuel behaviour, instead general tables or control variables are utilized. With those it is possible for example to determine the release of a radionuclide specie from fuel rods due to bursting during a transient or through pinhole leaks that develop due to erosion, fretting, or manufacturing defects in the fuel rod cladding or through leaching of the nuclide from the structural material in the reactor system [4, p. 3-19].
But the accuracy of this approach is not considered as adequate, because Relap5-3D is not capable of compute any material conversion of nuclear species during the runtime of the code.

2.4.2.2 Fission product (FP) transport model

A Eulerian radionuclide transport model is applied to simulate the transport of radioactive or fertile nuclides in the reactor coolant systems. In connection with the nuclear detector model this model can be applied to describe the response of the control and safety systems to the existence of radioactive species in the coolant systems. The radionuclide species may be transported by either the liquid or vapour/gas phases. It is possible to create a radioactive specie by either neutron absorption in a fertile specie or by injection into the coolant system using general tables or control variables [4, p. 3-19]. The concentrations of radionuclide species are assumed to be sufficiently dilute that the following assumptions are valid:

- The fluid properties (liquid or vapour/gas) are not affected by the presence of radionuclide substances.
- Energy absorbed by the transporting phase from the decay of radionuclide species is negligible.
- The radionuclide species are well mixed with the transporting phase so that they are transported at the phase velocity [4, p. 3-19].

Under these assumptions, the equation for the conservation of mass for a radionuclide substance is:

$$\frac{\partial C}{\partial t} + \frac{1}{A}\frac{\partial}{\partial x}(CvA) = S$$

Where

C… number density (concentration) of the radionuclide specie in atoms per unit volume (atoms/m^3),
v… velocity of the transporting phase,
A… cross sectional area of the flow duct
S… source of the radionuclide specie in units of atoms per unit volume per second [4, p. 3-19].

The number density (concentration) C may be converted to the mass density using:

$$\rho = \frac{C \bullet Mw}{N_a}$$

Where

ρ… mass density of the radionuclide specie in units of mass per unit volume (kg/m3),
N_a… Avogadro's number (atoms/kg-mole),
Mw… molecular weight of the radionuclide specie (kg/kg-mole) [4, p. 3-20].

2.4.3 Interlinkage to other codes in radiological consequences evaluation method

The code coupling capability is only available in some RELAP5-3D source code products [1,p. 2-1]. The coupling is done via the Parallel Virtual Machine (PVM) coupling Application Programming Interface (API) and the R5EXEC program, which controls and coordinates a coupled simulation [5, p. B-1]. The R5EXEC program is an overhaul of the PVMEXEC program used in earlier Versions of RELAP5-3D. It was introduced in RELAP5-3D Version 4.3.4 [9].

The coupling system shall enable the use of different codes for the simulation of different portions of the system in a unified analysis of the transient behaviour of the system. Data exchange is done using the Parallel Virtual Machine (PVM) message passing methodology, which can be done via locally on one computer or across a network on multiple computers. [5, p. B-1]

RELAP5-3D underwent major modifications to implement coupling capabilities and allow it to be part of coupled simulations [10] "*The original implementation of a PVM coupling interface was removed from the code and its control functionality was reproduced in the PVMEXEC code. This made the PVM coupling methodology independent of RELAP5-3D©. The original PVM coupling interface only implemented explicit parallel thermal-hydraulic coupling and new types of coupling were developed and implemented in the PVMEXEC code.*" [10, p. 2f]

"The basis of the coupling methodology as implemented by the R5EXEC program and by the R5EXEC Application Programming Interface (API) is domain decomposition. The domains that can be separated into separate pieces are the models of the important physical processes that determine the behavior of the system being simulated. The behavior of the separate pieces of the system being simulated are computed by different computer programs or by different instances of the same computer code. The physical processes that can be modeled by different computer codes are the thermal-hydraulic behavior of the fluids in the system, the neutronic behavior of the reactor core, the thermal-mechanical behavior of the solid structures in the system, and the behavior of the control components in the system being simulated. This means that one computer program may compute the behavior of the fluids in all portions of the system while other computer codes compute the neutronic behavior of the reactor core or the behavior of control components in the system." [11, p. 2]

More specific, synchronous and asynchronous thermal-hydraulic coupling, as well as synchronous kinetics coupling and synchronous control systems coupling have been implemented in the R5EXEC program [11, p. 3].

In the past R5EXEC was an underutilized tool in the RELAP5-3D which is believed to be largely due to the unavailability on Windows platforms [12]. While in theory, every code that implements the R5EXEC/PVMEXEC API may be used in a coupled simulation [5, p. B-1], there is almost no literature available on related coupling applications. Historically, the approach was rather to include the output manually in other programmes.

RELAP5-3D contains a basic routine which allows the user to plot calculation results. But the capabilities of the internal plotting package are not considered adequate for most applications. Thus, an external post-processing plotting routine is often used, for instance the software APT PLOT [8, p. 4-76].

2.4.3.1 Internal coupling with NESTLE

A multi-dimensional neutron kinetics model is included in RELAP5-3D based on the NESTLE code 7.0-2. Thus steady-state eigenvalue and time dependent neutron flux problems can be solved. [5, p. xiv].

2.4.4 Further development needs

Radioactive decay cannot be modelled adequately with RELAP5-3D [4, p. 3-19] as the code utilizes general tables or control variables to calculate fuel behaviour. It is only possible for the user to define which substances are present in which form (fluid/gaseous). But during the runtime of the code, the characteristics of the substances are not affected in any way. As a result, transported fission products do not experience any material conversion. In the R2CA project, it would be an important achievement if the radioactive decay could be included via an external model implemented into the RELAP5-3D radionuclide transport. Even though the radio chemistry would still be missing, the precise thermal hydraulic modelling that RELAP5-3D is providing (compared to integral codes) would outweigh the shortcomings in DEC-A transients.

2.4.5 References

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2.5 DYN3D

2.5.1 General overview of the code and modelling capabilities

DYN3D is developed for investigations of transients in cores of thermal power reactors with hexagonal or quadratic fuel elements [1], [2], [3].

The 3-dimensional neutron kinetics models of the code are based on a nodal expansion method for solving the two-group neutron diffusion equation in hex-z or rectangular x,y,z-geometry. Recently the code was extended to an arbitrary number of energy groups. Further, a simplified transport (SP_3) approximation for the flux calculation was implemented for fuel assemblies with quadratic cross section [4]. At present, the multi-group and the SP_3-version are part of a special DYN3D-version. It is foreseen to com- bine both versions in the near future.

The thermal-hydraulic (TH) part consists of a two-phase flow model describing coolant behaviour and a fuel rod model. The fuel elements are simulated by separate coolant channels. Additionally, some hot channels with power peaking factors belonging to chosen fuel elements can be considered. Several safety parameters such as temperatures, DNBR and fuel enthalpy are evaluated. The stationary state and transient behaviour can be analysed. To meet the conditions of the different users several different libraries of macroscopic cross sections are linked to the code.

DYN3D was validated by numerous benchmarks and experiments for thermal reactors with hexagonal and quadratic fuel assemblies. Concerning reactors with hexagonal fuel elements, the kinetic benchmarks defined by the Working Group D "VVER Safety Analysis" of Atomic Energy Research (AER) association were calculated. Considering reactors with quadratic fuel assemblies the code was verified by using the NEACRP Benchmarks on control rod ejections in PWR's and the NEA-NSC Benchmarks on withdrawal of control rods at hot zero power. The code has been coupled with the TH plant model ATHLET developed by GRS [5]. The coupled code was validated

with the help of AER benchmark for main steam line break (MSLB) in a VVER-440 (hexagonal) and the OECB-MSLB benchmark for the TMI-1 reactor which is a western type pressurized water reactor (PWR) with quadratic fuel assemblies. The boiling water reactor (BWR) turbine trip (TT) benchmark organized by the OECD and the American Nuclear Regulatory Commission (NRC) is based on the turbine trip test 2 of the BWR Peach Bottom 2. The experimental results and the results of the other participants at the benchmark were used for validation of DYN3D and the coupled version DYN3D/ ATHLET. Concerning VVER reactors DYN3D and DYN3D coupled with system codes have been validated in the frame of the project VALCO of European Union with the help of measured data at the nuclear power plant Bohunice (VVER-440) in the Slovak Republic and the VVER-1000 power plant Kosloduj (Bulgaria). The measurements at the W1000 test facility of the Russian Research Center "Kurtschatov Institute" have been used for the validation of the neutron kinetics of DYN3D.

2.5.1.1 Neutron Kinetics

The transient 3-dimensional neutron distribution is calculated by solving the time-dependent neutron diffusion equations for two energy groups and M groups of precursors of delayed neutrons with the help of nodal methods for hexagonal-z or Cartesian geometry. Dividing the reactor core into horizontal slices, the nodes n are the parts of the fuel assemblies in each slice. Considering the horizontal mesh in the Cartesian geometry the nodes can be subdivided, but not in hexagonal geometry. The thickness of the axial slices can be different. The neutron group constants are assumed to be spatially constant in each node n.

2.5.1.2 Core Thermo-Hydraulics Model

The model for the description of core thermo-hydraulics within DYN3D under steady-state and transient conditions is based on following principles:

- The core is represented by one-dimensional parallel coolant channels consisting of a fuel rod and the proportional coolant flow. Each coolant channel is connected to one or more fuel assemblies describing the average conditions. The channels are isolated, i.e. no cross flow between the channels is taken into account. The channels are coupled only over common boundary conditions. Furthermore, additional hot channels can be considered for analysing the effect of local power peaks, coolant temperature, flow rate or fuel rod parameters uncertainties.
- One- or two-phase flow can be considered. The description of two-phase flow is based on four differential balance equations for mass, momentum and energy of the mixture and mass balance of the vapour phase. The two-phase model is closed by the following additional assumptions:
    - One of the phases (vapour or liquid) is in saturation conditions. Its thermo-dynamic state is defined by the equation of state at saturation line.
    - The relation of phase velocities is described by a quasi-stationary phase slip model, that means, an algebraic equation for the phase slip ratio is applied.
- The thermo-hydraulic model is closed by constitutive relations for the slip ratio, oneand two-phase frictional pressure losses, evaporation and condensation rates, heat transfer correlations and thermo-physical properties of the phases.
- A fuel rod model considering one-dimensional heat transfer in fuel, cladding and within the gas gap between them is included. It is coupled to the flow model via heat flux at the cladding surface into the fluid.

The set of governing equations for the modelling of one- and two-phase adiabatic coolant flow is closed by so-called constitutive equations for:

- frictional and local pressure losses $\frac{\partial p_{fric}}{\partial z}$,
- heat transfer regime mapping including heat transfer correlations in different regimes and criteria for change of heat transfer regimes,
- evaporation and condensation rate (boiling model) and consistent phase slip correlation,
- mathematical formulations of the equations of state of water and steam including transport properties (thermo-physical properties package).

The correlations for the heat transfer coefficient (HTC) or one–phase liquid (laminar/turbulent natural or forced convection) and developed boiling heat transfer are chosen from [6].

The critical heat flux q''_{crit} is calculated by one of the correlations OKB-2 [7], [8], IAE-4 [9] or BIASI [10].

2.5.1.3 Fuel Rod Model

For the estimation of fuel and cladding temperatures, the heat conduction equation in one-dimensional radial geometry is solved. The parameters of the heat conduction equation can be temperature dependent. Parameters for the stationary reference state (e.g. geometrical gap width, gas pressure and composition) are given and have to be obtained from detailed fuel rod behaviour codes. The changes of the gas gap parameters during the transient process due to variation of gap width, gas temperature and pressure, coolant and fuel - cladding contact pressure are estimated by the model. In the gas gap between the fuel and cladding, the heat transfer components due to conduction in the gas, radiation and fuel–cladding contact are considered. In case of closed gap, heat transfer due to contact conductance is taken into account.

The main aim of the thermo-mechanical model is the estimation of gas gap conductance for a realistic temperature calculation. The simple thermo-mechanical model of the fuel rod is based on following assumptions:

- one–dimensional modelling of mechanics in radial direction,
- linear superposition of radial thermal, elastic and plastic deformations without axial coupling,
- elastic deformation of the fuel is taken into account only in the case of fuel–cladding contact, plastic deformations of the fuel are not considered,
- cladding is described in the thin shell approximation.

The thermal expansion of fuel and cladding is described by linear thermal expansion coefficients γ, which can be functions of temperature. The elastic deformation is proportional to the stress divided by the elastic modulus, which is also a function of temperature. The mechanical stress in the cladding is considered in the thin shell approximation, while for the fuel a hollow cylinder model is applied.

The gas pressure is obtained ideal gas law for the filling gas and taking into account change of gas temperature as well as change of free volume by change of gas gap width. For realistic estimation of depleted fuel rods behaviour, the change of gas pressure and composition due to fission product release during the transient has to be taken into account, but that has not been done in the present model.

The plastic deformation of the cladding is considered in accordance with the creeping law. Plastic deformation is considered, when the stress exceeds the yield strength, which is a material property and a function of temperature and strain rate.

Following assumptions are made for plastic creeping of the cladding in different cases:

- If the pressure outside the cladding (coolant pressure) is larger than inner pressure (contact pressure plus gas pressure), prompt creeping of the cladding on the fuel is assumed so that the gap vanishes and the cladding stress is zero. Contact pressure is obtained from this condition.
- If the pressure difference over the cladding is positive (inner pressure exceeds outer pressure), two different situations are considered:
    - If the gap is closed and contact pressure is non-zero, prompt creeping will be assumed until the stress is equal to the yield strength.
    - If there is no fuel – cladding contact and the gas pressure exceeds the coolant pressure, time-dependent creeping will be considered according with the creeping law.

The last situation is typical for low coolant pressures like in the RIA experiments at the pulsed research reactors or in LOCA cases and leads to cladding ballooning, while the first case is typical for RIA conditions in power reactors.

A deterministic model of fuel rod failure during accidents is not included in DYN3D, but some parameters for diagnostic of possible fuel rod failure are given, that are:

- fuel enthalpy for each axial node of the rod,
- cladding oxide thickness,

- signalization of possible cladding rupture, when the cladding stress is positive (inner pressure is larger than outer pressure) and exceeds the yield strength.

The metal-water reaction is considered as an additional heat source in the cladding, but the additional heat transfer resistance at the cladding surface and the change of mechanical properties of the cladding caused by the oxide layer are not taken into account (restriction to thin oxide layers).

2.5.1.4 Decay Heat Model

A model for calculating the space dependent decay heat power delivered from the operational history as well as during the transient is integrated in DYN3D.

The decay heat power is defined as the amount of thermal power released by the radioactive decay of fission and activation products. The contribution of the fission products to the decay heat power is calculated from the individual contributions of the four fissile isotopes ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu. The decay heat power delivered by each of these isotopes is divided into 24 groups having each a characteristic decay constant [11]. The decay heat power is calculated for the different nodes n in order to take into account its space dependence.

2.5.2 Fission product (FP) release and FP transport modelling in the code

DYN3D code does not contain mathematical models for simulation of FP release and/or transport.

2.5.3 Interlinkage to other codes in radiological consequences evaluation method

DYN3D and TRANSURANUS simultaneously prepare initial data for LOCA by each simulation of fuel rod behaviour history. LOCA transient is simulated by system TH code (RELAP), which results are further used as boundary conditions for fuel rod behaviour analysis in LOCA.

2.5.4 Further development needs

Further development/improvements of the realized models and methods are not supposed in the frame of the project.

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2.6 SHOWBIZ

2.6.1 General overview of the code and modelling capabilities

SHOWBIZ is a software studying the behaviour of a fuel cladding during its life, i.e. in reactor in normal operating condition (irradiation phase) or in accidental situations (RIA or LOCA), and outside the reactor vessel (transport or pool storage).

From a physical point of view, SHOWBIZ takes into account:

- the irradiation phase (cladding creep under irradiation),
- the thermal behaviour (computation the temperature field under various boundary conditions, in steady state or transient scenarios)
- mechanics including large deformation effects due to creep as well as the contact with neighbor objects,
- the diffusion of oxygen with crystallographic changes (metallic phases alpha, alpha+beta and beta, oxide phases monoclinic and tetragonal)
- the diffusion of hydrogen taking into account hydride precipitation/dissolution process with possible hydride radialization under stress,
- the effect of O and H concentrations on material properties,
- the transport/diffusion of an isotopic marker (O18).

SHOWBIZ can also manage various geometries, Cartesian or cylindrical 1D, 2D or 3D. Each model (thermics, mechanics, O diffusion, H diffusion) can be executed in stand-alone mode or coupled with any other models.

2.6.2 Fission product (FP) release and FP transport modelling in the code

The SHOWBIZ code do not model any fission product release and any fission product transport.

2.6.3 Interlinkage to other codes in radiological consequences evaluation method

The identified models on hydriding process for the behaviour of failed rods in SGTR conditions will be implemented in the SHOWBIZ software. SHOWBIZ is the IRSN "R&D" software dedicated to the modelling of the interaction between oxidation, hydriding and mechanical behaviour of the cladding. This tool is connected to the Fuel Performance code used by IRSN, FRAPCON. The envisaged methodology is based on a sequential coupling of FRAPCON and SHOWBIZ software.

- At first, FRAPCON will be used to compute the cladding properties induced by irradiation during a phase prior to the primary defect occurrence. Output from FRAPCON such as burn up, thermal flux, gap thickness will be considered as input for SHOWBIZ.
- Then a SHOWBIZ calculation will be performed in the aim to model the formation of secondary hydride region of failed fuel rods during normal operating conditions.
- Finally, a SHOWBIZ mechanical calculation will be performed to evaluate the mechanical strength of the embrittled fuel rods under SGTR transients. IRSN will use the CATHARE code in order to provide the coolant pressure evolution during the SGTR transient. These thermo-hydraulic conditions will define precisely the loading on the rods during the transient. The cladding ductility in presence of a secondary hydride region will be evaluated with SHOWBIZ. Mechanical approaches based on the linear elastic rupture can be applied.

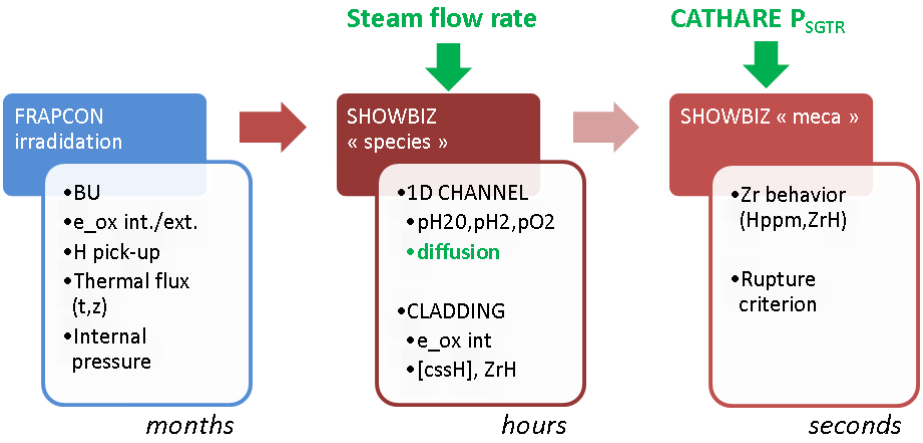

Figure 2.2. Sequential code coupling for secondary hydriding failure.

2.6.4 Further development needs

SHOWBIZ chemical calculation will be performed in the aim to model the formation of secondary hydride region of failed fuel rods during normal operating conditions. Specific developments have been identified and a 1D channel will be implement in order to take into account both gas transport in the gap and subsequent oxidation and hydrogen pickup at the inner surface of the clad. Hydrogen diffusion in the cladding thickness and eventually the formation of blister will be also implemented. In addition, failure criteria for hydrided cladding will be defined.

Finally, a SHOWBIZ mechanical calculation will be performed to evaluate the mechanical strength of the embrittled fuel rods under SGTR transients. The gradient pressure between the rod and the primary circuit is identified as a possible driving force for the failure of the secondary defective region

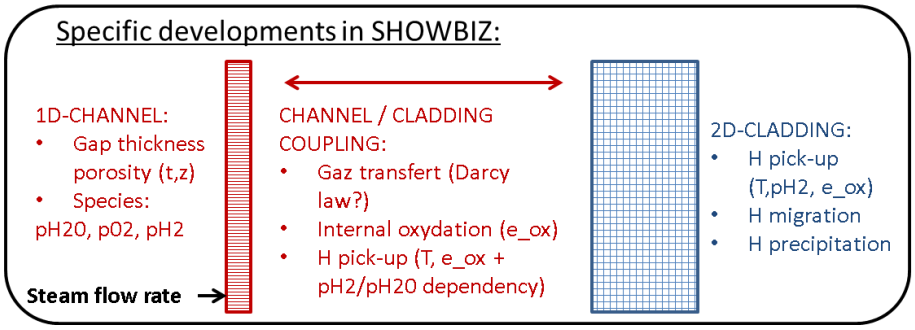

Figure 2.3. Specific developments envisaged in SHOWBIZ for secondary hydriding simulation.

2.6.5 References

No publication of the SHOWBIZ code is available in the literature because this code is developed since less than one year.

2.7 TRANSURANUS

2.7.1 General overview of the code and modelling capabilities

TRANSURANUS is a computer programme written in Fortran 95 for the thermal and mechanical analysis of fuel rods in nuclear reactors that is owned by the Joint Research Centre of the European Commission.

TRANSURANUS has been used by research centres, nuclear safety authorities, universities and industrial partners, (see Refs [1]-[15]).

TRANSURANUS is generally referred to as a fuel performance code meaning that it solves the equations for the radial heat transfer, the radial displacement along with the stress distribution in both the fuel and its surrounding cladding, and the release of fission product and its behaviour as a function of time. The equations, in general for fuel performance prediction, embody the following phenomena:

- Thermal performance: heat conduction, radiation and convection;
- Mechanical performance: creeps (radiation and high temperature), densification, thermal expansion, pellet cracking and relocation, solid and gaseous swelling;
- Actinide behaviour: depletion and build-up of main Th, U, Np, Pu, Am and Cm nuclides, impact on the radial power profile;
- Fuel restructuring: Pu and Am redistribution, grain growth (normal and columnar), central void formation;
- Fission product behaviour: creation in the fuel matrix, diffusion to grain boundaries, release to free rod volume after saturation of grain boundaries, athermal release, recoil, formation of High Burnup Structure (HBS, which is depleted and contain porosity).

The heat transfer in the fuel-to-cladding gap is simulated by means of a combination of heat conduction, radiation and convection (URGAP model [16]). Main assumptions and equations for mechanical performance are provided in Ref. [2].

Main assumptions and equations for actinide concentrations could be found in Refs [14], [15].
In the TUBRNP model the calculation of the radial power profiles is split into (a) the approximation of the neutron flux through thermal diffusion theory, and (b) the computation of the local concentrations of the relevant actinide isotopes with simplified depletion equations. The most recent extension covers the nuclides ^{232}Th, $^{233\text{-}236,238}$U, ^{237}Np, $^{238–242}$Pu, ^{241}Am, ^{243}Am, $^{242–245}$Cm. More details are given in Ref. [17].

The TRANSURANUS code consists of a well-defined mechanical and mathematical framework, which additional physical models can easily be incorporated. The code has a comprehensive material data files for oxide, mixed oxide, carbide and nitride fuel types, Zircaloy and steel claddings and several different coolants (water, sodium, potassium, lead, bismuth). TRANSURANUS can be used as a single code system for simulating both long-term irradiations under normal operating conditions as well as transient tests. The 'restart' mode allows simulating re-fabricated (recycled) fuel rods, where the fill gas has been completely changed as an example.

The code can be employed in two different approaches: as a deterministic or a statistical code. Restart may be used to perform a statistical analysis employing the Monte Carlo technique. This option may be helpful for the analysis of a long base irradiation then followed by a transient.

Besides its flexibility for fuel rod design, the TRANSURANUS code can deal with a wide range of different situations, as demonstrated in experiments, under normal, off-normal and accident conditions, although some models specific for RIA (e.g. plenum temperature) are still under development. Furthermore, the code is being used for BWRs, PWRs and VVERs. The time scale of the problems to be treated may range from milliseconds to years. Hence complex irradiation experiments can be simulated including re-fabricated instrumented fuel rods and changing operating conditions.

2.7.1.1 Basic assumptions and models

The basic assumptions and models can be summarised as follows:
Thermal analysis:

- Steady-state and transient analysis
- Phase changes included
- Advanced numerical solution technique (fast and stable)

Mechanical analysis:

- Constitutive equations
- Equilibrium
- Compatibility
- Superposition of one-dimensional radial and axial mechanical analyses

This mechanical concept leads to a semi-analytical solution, which is solved by an effective numerical algorithm.

Physical models:
All important physical models are included, i.e. models for thermal and irradiation-induced densification of fuel, swelling due to solid and gaseous fission products, creep, plasticity, pellet cracking and relocation, oxygen and Pu redistribution, volume changes during phase transitions, formation and closure of central void and treatment of axial friction forces.

2.7.1.2 Verification

The verification was performed by the following steps:

- Verification of the mechanical–mathematical framework by comparison with exact solutions, which are available in many special cases (analytical verification), and by comparison with different solution techniques, which were applied in order to optimise the numerical analysis
- Extensive verification of models
- Verification by code-to-code comparisons with many different codes
- Verification by comparisons with experiments: LWR and FBR fuel pins were extensively verified under steady state conditions, the FBR version was verified for less cases [18].

2.7.1.3 Current status

The capabilities of the TRANSURANUS code can be summarised as follows:

- Analysis of all fuel rod types under normal, off-normal and accident conditions (deterministic and probabilistic) is in principle possible.
- Consistent steady-state and transient analysis
- Clearly defined mechanical-mathematical framework into which physical models can easily be incorporated
- Fast and reliable
- Database, models and code extensively verified
- Applied by different groups and different licensing authorities

2.7.2 Fission product (FP) release and FP transport modelling in the code

There are different models for fission gas behaviour available in the TRANSURANUS code. The standard fission gas release model of TRANSURANUS can be described in a serial way.

1. The fission gas is created. This amount is derived from the linear power indicated as input after converting it to a volume power generation rate, the type of fuel and the type of neutron spectrum. A limited number of elements are considered: Xe, Kr, Cs, Nd and He.
2. The intragranular routine calculates the amount of gas that reaches the grain boundaries. This is done using the various numerical solutions for the Speight model, including a modified algorithm developed for example by Forsberg and Massih or the URGAS model. It is usually assumed to be the same for xenon and krypton as the literature is too scarce and uncertain to use different ones.
3. A fraction of the initial porosity resulting from fabrication is considered to be open porosity.
4. This open porosity is converted to the surface fraction of the grain boundaries covered by open porosity.
5. A fraction of the gas reaching the grain boundaries, corresponding to this surface fraction of open porosity, is directly released to the volume. It is therefore removed from the gas stored at the grain boundaries.
6. The grain boundary sweeping routine is activated.

7. The high burn-up routine is optionally launched.
8. The intergranular routine determines if the gas stays at the grain boundary or is released to the open volume, i.e. whether the grain boundaries are saturated or not.

The steps 3, 4 and 5 replaces a single step consisting of releasing a fraction of the fission gas produced between the steps 1 and 2. However, this work is under development and has not yet been included in the standard version of the code. A recent review of the fission product behaviour modelling can be found in [19].

2.7.3 Interlinkage to other codes in radiological consequences evaluation method

In the frame of the ESSANUF project, various codes were coupled with the TRANSURANUS code: ATHLET, RELAP, SERPENT and DYN3D [20]. For LOCA analysis, DYN3D and TRANSURANUS simultaneously prepare initial data by each simulation of the fuel rod behaviour history. The LOCA transient is simulated by system thermal-hydraulic code (RELAP), which results are further used as boundary conditions for fuel rod behaviour analysis in LOCA.

2.7.4 Further development needs

General needs for fuel performance codes have been reviewed in a recent review paper [21]. In the frame of R2CA, the JRC will be involved in developments of models for the hydrogen uptake under DBA conditions and redistribution in the cladding, based on work carried out in the frame of bilateral agreements for TRANSURANUS licenses. The model for hydrogen uptake will consider in a first step an assessment of models for hydrogen uptake by Zircaloy at high temperatures (e.g. during LOCA conditions) available in the open literature. A stand-alone model for hydrogen uptake of Zr1%Nb cladding and its effect on the oxidation and mechanical strength were addressed in the wake of the incident at the Paks NPP in 2003, indicating that the hydrogen uptake plaid a significant role in the mechanical deterioration of the cladding material. In line with the high temperature oxidation model, the content of hydrogen uptake is computed incrementally with a quasi-stationary approach. Different model constants were applied for varying conditions (e.g. steam oxidation or steam starvation oxidation conditions). Based on the literature study, the most suited model will be implemented in TRANSURANUS and merged with the model for hydrogen uptake under normal operation conditions. JRC will perform independent testing and verification of the model.

Another hydrogen related modelling work will consider radial hydrogen redistribution in the cladding, and that will also be done within a TRANSURANUS bilateral licence agreement, followed by JRC's independent testing. The work starts with a literature review. Hydrogen absorbed in zircaloy may redistribute and precipitate as brittle hydride platelets, which can severely degrade the cladding ductility. Under a heterogeneous temperature distribution, hydrides tend to accumulate in colder areas, creating local spots of degraded cladding that can favour crack initiation. Therefore, an estimation of the local hydride distribution is necessary in order to predict the risk of cladding failure, as well as for consideration of its effect on the mechanical properties. Hydride distribution is governed by three competing phenomena. Hydrogen in solid solution diffuses under a concentration gradient due to Fick's law and under a temperature gradient due to the Soret effect. Precipitation of the hydride platelets occurs once the hydrogen solubility limit is reached. The model development for TRANSURANUS will make use of existing models in the code that consider similar processes (e.g. Soret effect) in cylindrical geometry such as existing models for oxygen, plutonium and actinide redistribution (OXIRED, PUREDI, AMREDI) [22-24]. The model for the hydrogen distribution in TRANSURANUS will be compared with the results published in the literature.

JRC will implement new models in the current version of the TRANSURANUS code to describe the influence of the hydrogen content on the creep behaviour of Zircaloy-4 cladding tubes, on the basis of previous work carried out at the Technical University of Münich for E.ON. The former developments were made in Fortran77 and were based on calorimetry and dilatometry data that were used to modify the static and dynamic phase transfer models of TRANSURANUS. The new phase transfer models should be able to be applied for temperature gradients between -100 and +100 $C.s^{-1}$ and for hydrogen contents up to 1000 ppm. The Zircaloy-4 creep model has been calibrated on isothermal burst experiments performed for hydrided and non-hydrided specimens. For that purpose, Norton creep parameters (structure parameter, stress exponent) have been adopted in each crystallographic phase domain. The new models should allow to assess the increase of damage extent due to the influence of the

hydrogen in Zircaloy-4. Nevertheless, on this basis new correlations for other cladding tube materials can be implemented easily in order to take into account the influence of hydrogen.

JRC will also implement the ANS5.4 model [25] for radioactive fission product release. The implementation to the latest code version will be done based on previous work done elsewhere [26]. This model provides a methodology for determining the radioactive fission product releases from the fuel for use in assessing radiological consequences of postulated accidents that do not involve abrupt power transients. When coupled with isotopic yields, this method establishes the "gap activity," which is the inventory of volatile fission products that are released from the fuel rod if the cladding is breached. The isotope that provides the most significant contribution to equivalent dose to individuals is generally I-131 for accidents that occur during in-reactor operation or shortly after reactor operation. The ANS-5.4 model predicts the release of radioactive fission products Xe, Kr, I, Cs and Te into the rod free volume from the fuel matrix. As far as physical phenomena is concerned, the model is based on diffusional release in a spherical grain like the original Booth model, but it also simulates bubble interlinkage and formation of tunnels through a step in the surface-to-volume ratio. As interlinkage occurs, the grain boundary bubbles gain a direct connection to the free volume. The surface-to-volume ratio is an empirical function of local temperature and burnup.

POLIMI targets to implement an updated version of the ANS5.4 model into POLIMI's in-house fission gas behaviour module SCIANTIX, and couple the module with TRANSURANUS. SCIANTIX will also be added with modelling of high burnup structure formation and evolution which are important concerning the contact pressure between the fuel and the cladding and thus the potential failure by secondary hydriding. It is proposed to modify the ANS5.4 model by considering the grain boundary coverage fraction defined in state-of-the-art mechanistic models for inert gas behaviour, substituting the semi-empirical approach based on tuning of the surface-to-volume ratio of the fuel grains, and by revising the semi-analytical numerical treatment adopted in the original ANS5.4 with incremental numerical solution of governing differential equations, in line with the other models in the code. These activities ensure that the model describing the release of radioactive fission products is going to be consistent with state-of-the-art modelling of fission gas release, and therefore the modelling of fission product release can leverage mechanistic model developments already available for fission gas description, e.g., additional release due micro-cracking of grain boundaries during transients.

IRSN will extend the existing TRANSURANUS/MFPR-F coupling in order to take better advantage of the capabilities of both codes. Firstly, IRSN will make the suitable adaptations so that the HBS model of MFPR-F can be activated in the coupling. Secondly, the coupling will be extended to oxidising conditions following cladding breach, provided that the oxygen potential in the gap can be derived from the model for axial gas evolution developed for failed fuel by UJV (see below).

ENEA will extend the TRANSURANUS code in R2CA related to the effects of the hydrogen uptake on the M5 cladding material properties and on cladding burst models relevant for LOCA. More precisely, ENEA will modify the models and material properties for high-temperature creep, the phase transition model and the burst criterion to account for the effect of hydrogen in the TRANSURANUS code calculations for assessing the number of failed rods under LOCA conditions for M5 cladding. This work will rely on information provided in the open literature.

UJV will enhance the capabilities of the TRANSURANUS code with models concerning some phenomena which are not treated in the code to date, but which may impact the fuel rod behaviour during the LOCA according to the experimental data. There are two main areas which will be addressed. The first one is the transport of the gas in the rod before burst. The current models expect instantaneous equalization of the pressure between all free volumes in the fuel rod. This mostly results in a single balloon being predicted at the hottest axial elevation of the rod. However, recent experiments with longer rods suggest that more than one balloon may form and burst on a single rod. The plan of the work is to benchmark standalone numerical model to ABAQUS-CFD or MELCOR/RELAP/CATHARE calculation, and then implement it to TRANSURANUS. The second development area is the transport of the gas in the rod after the burst. In order to assess the location and extent of the secondary hydriding, it is necessary to not only add the models of the oxidation and hydriding of the cladding internal surface, but also to take into account the diffusional mixing of the gases along the fuel cladding gap. Standalone model will

be developed, benchmarked with ABAQUS calculation, and then implemented and tested. Furthermore, UJV will improve the modelling of the fuel temperature in failed rods. Fuel temperature is driving the fission product release regardless of the applied release model. UJV plans also to further develop statistical calculation sequence between RELAP5 or ATHLET and TRANSURANUS.

NINE will implement correlations from open literature into TRANSURANUS considering analytical models for the prediction of FGR from defective fuel. This modelling takes into account the size of the defect and key mechanisms.

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2.8 DRACCAR

2.8.1 General overview of the code and modelling capabilities

DRACCAR [1] is a multi-rod code developed by IRSN since 2006 to predict thermo-mechanical fuel behaviour during LOCA accidents including 3D two-phase flow modelling with evaluation of reflooding efficiency. The main objectives of the code are to help analysing and understanding experiments and providing alternative to thermal-hydraulic (TH) system code to propose insights on safety criteria relevance. DRACCAR software belongs to the IRSN FUEL+ platform which gathers the knowledge on fuel behaviour in normal and accidental conditions.

DRACCAR is a coupling platform between a structure code [2], ICARE3D and a TH code, CESAR (developed at IRSN) or CATHARE 3 (developed by CEA) [3]. These two main codes are connected to auxiliary modules (developed at IRSN) that deal with database management, material properties, scenario management and decay heat calculation. A schematic view of this structure is illustrated in Fig. 2.4. The material properties databank MDB is very flexible and allows adding new materials easily (properties as well as physical behaviour laws). An implicit numerical scheme couples the thermo-mechanical code to the 3D TH. In addition to 3D core domain, the modelling can be completed by the description of the cooling circuits and systems (primary loop, SGs, emergency systems) by the TH code. Thus, the whole coolant circuits can be simulated within DRACCAR application.

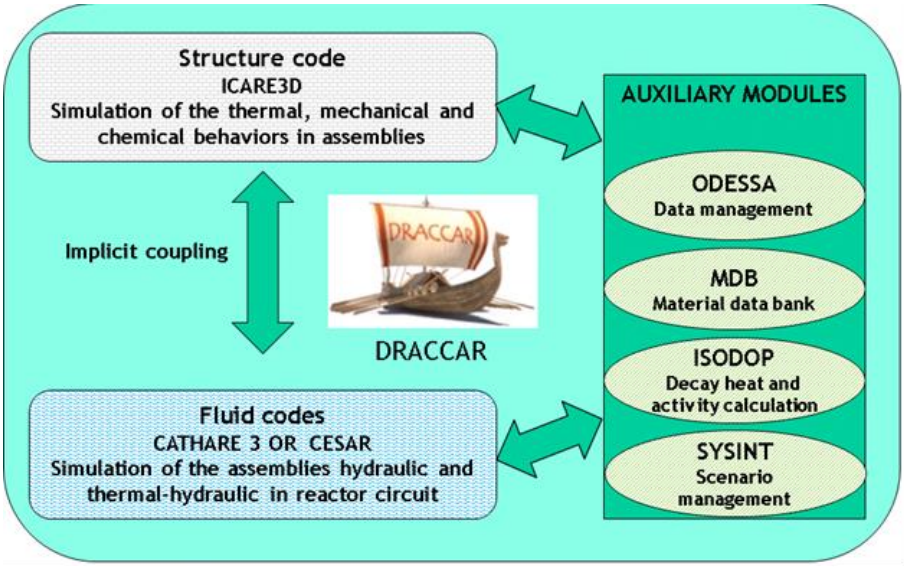

Figure 2.4. Codes and modules available in the DRACCAR platform.

ICARE3D, the thermo-mechanical code used in DRACCAR computes thermal, thermo-mechanical and chemical behaviour of fuel assemblies. Several rods can be modelled and discretized axially, radially and azimuthally and located in a 3D TH meshing. ICARE3D deals with the main heat exchanges: conduction inside a structure and between structures in contact, radiation/conduction in gap between the fuel and the cladding, radiation between rods or rod/shroud, convection between the structures and the two phase flow. In addition, specific treatment of reflooding is carried by a dedicated model evaluating the quench front progression and associated strong heat exchanges.

The thermo-mechanical behaviour of Zr alloy cladding uses a quasi-3D approach with diagonal stresses and strains (shear or bending are not taken into account). The code takes into account contacts between structures (by freezing the cladding node location without sliding). The strain is assumed to be a linear superposition of thermal and creep strains (for cylinder-like structures). Only secondary creep is modelled, by a Norton law, whose coefficients depend on the crystallographic phase of zirconium alloy. Different burst criteria on strain, stress and cumulated strain are available. The strain and cumulated criteria are derived from two experimental databases, the NUREG-0630 or the French EDGAR programme. The stress criterion is also derived from the EDGAR programme [4].

The deformation of rods and the progressive blockage of fluid channels are evaluated all along the transient. Therefore the influence of blockage on 3D flow deviation and on the convective heat exchanges is computed in the same time line using an implicit scheme for the coupling of thermo-mechanics and TH. This can be done in multi-rods configuration with the help of an optimized numerical method. In addition shared memory parallelism can be used.

Regarding the fuel behaviour in LOCA conditions, DRACCAR proposes a parametric axial fuel relocation model which represents fuel fragment relocation within the cladding balloon. It can be used to gather knowledge through sensitivity studies accounting for the increase of local power in the ballooned zone. The model principle is to trigger the axial relocation of fuel on user input criteria (threshold strain value, burst timing…) and to move fuel from stacks above to fill free space consistently with the filling ratio set by the user. Moreover, the fuel model description is progressively improved for instance by the development of a 1D-axial gas transport model.

An extensive validation database has been constituted over the years containing the most relevant separate-effect tests and integral tests concerning LOCA [5]. The TH validation database is constituted of several tests from more than ten experimental programmes (PERICLES, ROSCO, FEBA, KIT, SEFLEX, THETIS, ACHILLES…) and mainly focused on reflooding phenomena in both intact and deformed geometries. The thermo-mechanical

validation is based on the EDGAR programme and on integral tests (PHEBUS LOCA, Halden IFA-650, REBEKA, QUENCH LOCA, NRU MT-3, etc).

Fig. 2.5 illustrates an example of simulation corresponding to the PHEBUS LOCA test 218 with the DRACCAR code. All the facility is modelled (multi-rod modelling of the bundle test section and modelling of the TH circuits connected to test section). The entire transient (blowdown, refilling and reflooding phases) is reproduced.

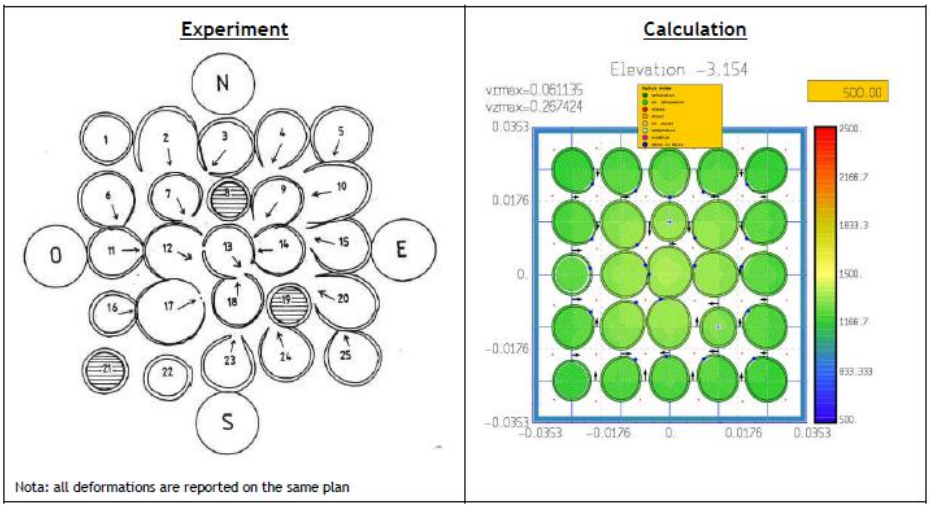

Figure 2.5. Cladding deformation at the end of the transient in the PHEBUS 218 test– DRACCAR simulation-experiment comparison.

The context of development of the DRACCAR platform is strongly linked to the PERFROI experimental programme [6], which includes three different experimental projects. The COAL project is dedicated to the study of reflooding in a deformed fuel bundle using electrically heated fuel rod simulators, paying special attention to represent correctly the power profile and thermal inertia in the blocked zone. The COCAGNE experiments investigate rod deformation, the mechanical interaction with neighbours, and rod burst. The ELFE experiment aims to characterize material creep and failure behaviour on cladding samples in a heated stress machine device. This PERFROI programme will generate data to help develop and validate the DRACCAR platform concerning the mechanical and TH behaviour of fuel rods under LOCA conditions (cladding deformation, mechanical contact amongst rods, cladding failure, reflooding of representative deformed fuel rods with an increase of the power in the ballooned region due to fuel relocation). In addition, the DRACCAR development perspectives include other topics such as fuel fragmentation and relocation, and gas transport and fission product release during LOCA which are investigated through the OECD Halden and OECD SCIP-III projects and in upcoming projects, such as VERDON LOCA by CEA Cadarache.

2.8.2 Fission product (FP) release and FP transport modelling in the code

The DRACCAR code do not model any fission product release and any fission product transport.

2.8.3 Interlinkage to other codes in radiological consequences evaluation method

DRACCAR is currently not able to depict a whole core - except by using a standard approach based on averaged weighted rods which cannot lead to a detailed evaluation on fuel rod behaviour. In the frame of R2CA, DRACCAR capabilities will be extended to the description of the whole core coupled to reactor primary and secondary loop. It means that core domain will not be limited to a weighted single equivalent fuel assembly or only to average weighted rods located in TH core rings. This approach will mix modelling scales with fined assembly description at sub-channel scale as well as coarser meshing using lumped volume and equivalent weighted rods to depict other part of the core. Both scales will be managed in a single simulation proposing the whole core response to LOCA. This work should lead to propose new type of applications able to take into account more in depth the behaviour

of some fuel assemblies and their interaction with the rest of the core. In a further step, the core domain will be included in a whole reactor circuit simulation (RPV, primary and secondary loops).

The DRACCAR code will be linked to the TH code CATHARE code which will provide boundary conditions of the LOCA scenario, and to the ASTEC code in order to assess the transport of the FP in the primary circuit, in the containment and finally the Radiological Consequences.

The coupling between CATHARE and DRACCAR is operational. However, DRACCAR and ASTEC are not yet coupled. It is expected to develop an external coupling between both codes.

2.8.4 Further development needs

One of the targets for the development of the DRACCAR platform concerns the simulation of LOCAs with the modelling of a large number of fuel assemblies. Multi-scale modelling activities are investigated in the framework of research and development associated with the DRACCAR platform to allow the detailed assessment of the behaviour of a fuel assembly by taking into account the interaction with neighbouring fuel assemblies. In such applications, a zoom on a group of fuel rods is done using a fine multi-rod meshing. Other fuel rods belonging to the core are also modelled using a weighted averaged single rod approach inside each homogenized cells of a coarser meshing. Of course, such application requires a high-performance numerical approach and specific verifications and validation of the interactions between the fine and coarse meshings with transition rules between scales to obtain a consistent description. Both scales will be managed in a single simulation proposing the whole core response to LOCA. This work should lead to propose new type of applications able to take into account more in depth the behaviour of some fuel assemblies and their interaction with the rest of the core. In a further step, the core domain will be included in a whole reactor circuit simulation (RPV, primary and secondary loops).

2.8.5 References

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2.9 FRAPTRAN

2.9.1 General overview of the code and modelling capabilities

FRAPTRAN is a single-rod transient fuel performance code developed by Pacific Northwest National Laboratory (PNNL) for the U.S. Nuclear Regulatory Commission (NRC) [1]. FRAPTRAN has been written with Fortran language, and it is intended for modelling various transients and accidents such as LOCA, reactivity-initiated

accident (RIA) and anticipated transient without scram (ATWS). FRAPTRAN applies finite difference solution and axially stacked pellet and cladding slices with radial noding, commonly known as the 1.5 dimensional approach, i.e, the axial slices are coupled only by the rod internal pressure and coolant conditions.

FRAPTRAN calculates heat conduction in the pellets, cladding-to-coolant heat transfer, deformation of the pellets and cladding, cladding oxidation, and evolution of fuel rod internal gas pressure. There is also a transient fission gas release (FGR) model but that is validated only on RIA experiments. The code can be used to evaluate cladding failure time, axial location of the ballooning, failure temperature, cladding residual strain and high temperature oxidation, and it can be used to plan and analyse the results of LOCA tests in research reactors and out-of-reactor test devices. Fuel fragmentation behaviour is not considered in the standard version of FRAPTRAN but has been included for instance by SSM [2] to a special version of the code. FRAPTRAN's validation against LOCA experiments is described in [3]. FRAPTRAN does not calculate steady-state irradiation phase but this information is given via a restart file calculated with the FRAPCON code [4] from the same code family.

Uncertainty and sensitivity analyses can be made with the code as various model parameters can be varied through the input file: there are multipliers for cladding thermal conductivity, thermal expansion, yield stress and surface heat transfer coefficient, and for fuel thermal conductivity, thermal expansion and specific heat. FRAPTRAN does not support parallel execution but it is relatively fast running due to the 1.5 dimensional approach, and sequential runs for the uncertainty analysis can easily be done.

The FRACAS-I mechanical model for the fuel and cladding is the same as used in FRAPCON. For the fuel, it is a so-called rigid pellet model, i.e., it does not consider stress-induced deformation of the fuel. As soon as the cladding ballooning starts in one axial node, FRACAS-I model is no longer used in any node. FRAPTRAN and FRAPCON have common fuel and cladding thermal and mechanical material properties [5]. The temperature range of material properties is from room temperature to melting [1].

For high temperature oxidation, FRAPTRAN originally has two alternative models, Cathcart - Pawel (C-P) and Baker - Just (B-J) [1]. The C-P and B-J models activate if the cladding temperature exceeds 800°C and 727°C, respectively. The C-P model is recommended instead of B-J if the maximum cladding temperature is not foreseen to exceed 1527 °C [1]. Further models describing the high-temperature steam oxidation of the Russian cladding E110 (Zr1%Nb) between 600 °C and 1200 °C have been implemented into the code by EK [6].

The default LOCA cladding failure criterion in FRAPTRAN is explained as follows. The BALON2 ballooning model of FRAPTRAN assumes that local non-axisymmetric cladding ballooning begins when the effective plastic strain in any axial segment of the cladding exceeds the instability strain given by the material properties package MATPRO [7]. FRAPTRAN predicts the fuel rod failure in the ballooned region when the calculated true hoop stress in the cladding exceeds an empirical limit, or when the cladding plastic hoop strain exceeds a strain limit [1]. In the stress calculations, FRAPTRAN takes into account the thinning of the cladding resulting from the high temperature oxidation. The stress criterion is fitted using Zircaloy data, and it is applied for Zircaloy-2, Zircaloy-4, ZIRLO™, Optimized ZIRLO™ and M5™ claddings [1]. Furthermore, preliminary criteria describing the failure of the E110 cladding (Zr1%Nb) have been added by EK (n.b., no public references available yet).

The integral assessment database [3] of FRAPTRAN consists of 43 in- and out-of-reactor test cases. However, there are only ten LOCA cases, and three of those use pre-irradiated fuel (with 44, 56 and 83 MWd/kgU rod average burnup), tested in Halden. The other assessment cases are from the following test facilities: NRU (three cases), PBF (three cases), and TREAT (one case) [3].

2.9.2 Fission product (FP) release and FP transport modelling in the code

FRAPTRAN can be used to calculate transient FGR but currently the model has been assessed only against RIA experiments done in CABRI and NSRR research reactors [3]. Another option for the user is to give the evolution of FGR for FRAPTRAN as an input, in order to take it into account in the internal gas pressure evolution and composition used in thermo-mechanical predictions.

The distribution of fission gases in the pellets (radial, inter- and intragranular) prior to the transient is given by the FRAPCON code and its FRAPFGR model. It should be noted that the default FGR model in FRAPCON is the Massih model which is also recommended by PNNL, but it cannot provide the information on distribution of fission gases. The transient FGR in FRAPTRAN is temperature dependant as follows [1]: all grain boundary gas from a radial node is released when the temperature exceeds 1093°C; all gas from the restructured grains in the high burnup structure in a radial node is released when the temperature exceeds 1816°C; 5 % of the gas in the unrestructured grains from a radial node is released when the temperature exceeds 1816°C.

As FRAPTRAN is a fuel performance code, it does not consider FP transport beyond the fuel rod domain. However, studies on dispersal and mobility of fuel particles based on FRAPTRAN analyses have been conducted [8, 9].

2.9.3 Interlinkage to other codes in radiological consequences evaluation method

FRAPTRAN uses time-dependent fuel rod power and coolant conditions as its boundary conditions. Coolant behaviour can be pre-calculated by an external system or thermal hydraulics (TH) software and be given as input. U.S. NRC uses TRACE for this purpose [10], and in R2CA the Apros [11] system code is applied by VTT. There are two options for giving the coolant boundary conditions for FRAPTRAN. In the first option, coolant pressure and mass flux evolutions as well as the inlet, outlet or average enthalpy are given. The channel geometry is also defined. The heat transfer correlations are applicable for both PWR and BWR accident conditions [1]. In the other option, axial profiles of coolant temperature and cladding-to-coolant heat transfer coefficients are given, as well as the coolant pressure evolution. The latter option is convenient, for instance, if the cladding outer surface temperature is prescribed (calculated by another code, fixed in the experimental sequence, etc.).

Furthermore, FRAPTRAN can be coupled with an external TH software. At VTT, FRAPTRAN has been coupled [12] with VTT's in-house sub-channel TH code GENFLO [13] for improved TH modelling. In that case, Apros is used to provide the boundary conditions for GENFLO. Statistical LOCA analysis with the calculation system (Fig. 2.6) is described in [14-17], and sensitivity analysis of local uncertainties in LOCA simulations in [14, 18].

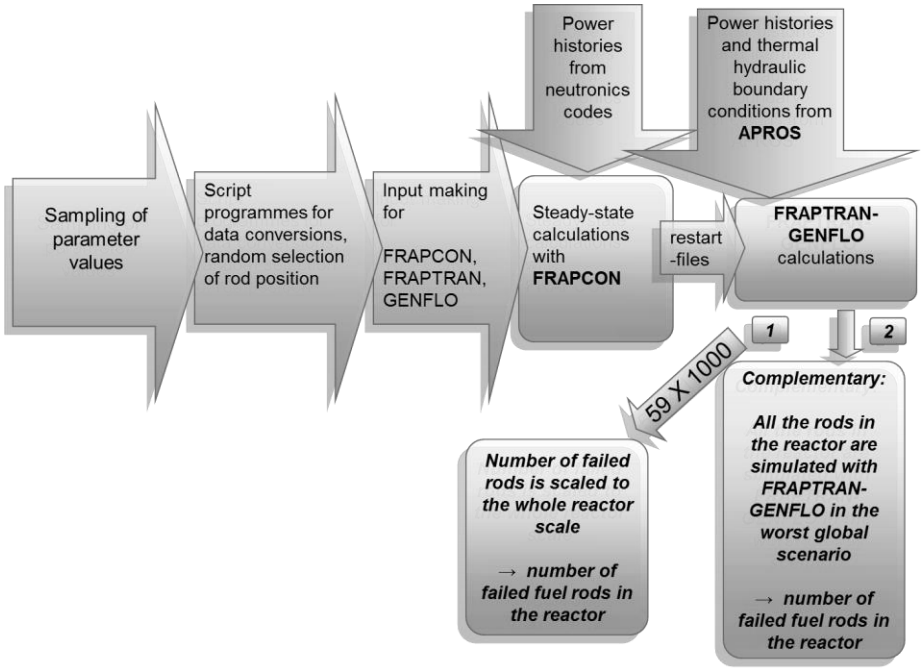

Figure 2.6. Number of failing fuel rods in LOCA is evaluated at VTT with the coupled FRAPTRAN-GENFLO using the base irradiation history from FRAPCON and transient boundary conditions from the system code Apros.

2.9.4 Further development needs

Experimental database on cladding failure in LOCA will be re-assessed in R2CA in order to improve the LOCA cladding failure predictions made with FRAPTRAN. As a result, more accurate cladding failure predictions are expected.

2.9.5 References

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2.10 MFPR-F

2.10.1 General overview of the code and modelling capabilities

The MFPR-F code (Module for Fission Product Release - France) describes mechanistically the fission product (FP) behaviour in intact UO_2 fuel under irradiation regimes, annealing regimes and accidental situations [1]. It is extensively validated against separate-effect tests, semi-analytical out-of-pile tests and large-scale in-pile tests [2]. MFPR-F is based on the MFPR code which was developed by IBRAE in collaboration with IRSN (IBRAE: models and code development; IRSN: code application to interpretation of FP behaviour and benchmarking). Since 2011, the code has been developed independently by both institutes.

One of the main strengths of the MFPR-F code is the consideration of microscopic defects in the UO_2 crystal structure, and of the multicomponent, multiphase system of chemically active FP including, in particular, solid precipitates. Both phenomena can strongly influence FP transport out of grains and release from fuel pellets in transient and/or annealing conditions.

2.10.2 Fission product (FP) release and FP transport modelling in the code

It is assumed that FP elements are originally generated in the UO_2 matrix in atomic (or ionic) form. All atoms formed by fission processes migrate to grain boundaries. In this way, fission gas atoms can form intragranular gas bubbles in which they might be further trapped. These bubbles can also migrate to grain boundaries. Part of the captured atoms can escape from bubbles by irradiation-induced and thermal re-solution processes. Point defects (vacancies and interstitials) and dislocations are also formed by fission processes in UO_2 matrix, mutually interacting with each other and with gas bubbles and as-fabricated pores.

Chemical interactions between the FP elements and the dissolved oxygen result in formation of separate phases in solid precipitates on the grain boundaries and vaporisation to the intergranular gas bubbles considered as the major mechanism for release of the fission products. Since distribution of elements depends significantly on the oxygen potential of the system, a model for fuel oxidation in steam/air mixtures was also developed. Processes of vapour formation affect significantly the release rates of all FP elements including noble gases.

Intergranular bubbles are represented by two groups: bubbles on grain faces (GF) and on grain edges (GE). The GF bubble growth progresses up to the grain surface saturation, when interlinkage of the GF bubble and formation of grain face channels to the grain edges occurs. Growth of the GE bubbles leads to their interconnection by tunnels and formation of an open porosity structure.

The accumulation of dislocations in UO_2 matrix during irradiation leads to the formation of the high burnup structure (HBS), characterized by sub-micronic grains and large pores filled with noble gas and volatile FP. A model for release of those FP during thermal transient accounting for over-pressurization of HBS pores was developed.

2.10.3 Interlinkage to other codes in radiological consequences evaluation method

The MFPR-F is coupled to the fuel performance code TRANSURANUS [3]. It is called, via an Application Programming Interface, in each TRANSURANUS mesh as module for FP behaviour, using temperature, hydrostatic pressure and fission rate density as inputs. The fission yields of some elements calculated by TRANSURANUS are also transferred. The variables returned by MFPR-F to TRANSURANUS are FP amounts in in UO_2 grains and in intergranular bubbles, FP release and grain size. The other MFPR-F outputs concerning microstructure and FP chemistry are also available in the coupling.
Apart from temperature, hydrostatic pressure and fission rate density, MFPR-F also requires the gas composition in the vicinity of the pellet to be provided for the model of fuel oxidation in steam/air mixtures.

2.10.4 Further development needs

In the HBS model of MFPR-F, the FP release is based on an arbitrary bubble pressure threshold. A more mechanistic approach would require a model accounting for the mechanical process of fuel cracking under HBS pore overpressurization. Thanks to recent developments, the MFPR-F code takes into accounts the formation and growth of HBS during irradiation, and the FP release during thermal transients. This model is already available in MFPR-F but it does not account for the effect of cladding restrain. The recent coupling of MFPR-F with the fuel performance code TRANSURANUS will address this issue. IRSN, along the R2CA project, will make the suitable adaptations so that the HBS model of MFPR-F can be activated in the coupled code

The impact of fuel leaching by water on FP chemistry is not taken into account in MFPR-F. The coupling between the MFPR-F code and the TRANSURANUS code of the JRC will be extended to oxidising conditions following cladding breach, provided that the oxygen potential in the gap can be derived from the model for axial gas evolution developed for failed fuel by UJV (see Section 2.7).

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2.11 TSKGO

2.11.1 General overview of the code and modelling capabilities

The TSKGO computer code simulates the activity release from leaking fuel rods. The code calculates the activity inventory in the free volume of the fuel rod and estimates the release of different gaseous and volatile fission products during steady state operation in the reactor, storage in the spent fuel pool and transient (e.g. sipping test) conditions. The calculated results show that the activity release during sipping tests is driven by the expansion of the gas volume inside the fuel rod and the amount and composition of the released radioactive isotopes highly depend on the defect location.

The TSKGO program can simulate the whole history of the fuel elements. This is necessary because the activity release during the examination highly depends on the amount of fission products accumulated in the free volume of the rod. The simulation starts from start-up of the reactor with the simulated fresh fuel rod. Activity releases during normal operation, shutdown procedure, storage in the spent fuel pool and manipulations including sipping tests are also simulated by the code. The calculated period can be several years covering the fuel cycles of the given fuel assembly and its long term storage in the spent fuel pool

2.11.2 Fission product (FP) release and FP transport modelling in the code

The TSLGO code calculates the amount of fission products in the free volume of a single fuel rod considering the following four processes:

- release of the fission products from the fuel pellet into the free volume,
- release of the fission products from the gap into the coolant through the defect,
- radioactive decay and
- birth due to the decay of precursor nuclei found in the free volume

The code can simulate the transport of several gaseous and water-soluble fission products, including radioactive (^{84}Br, ^{87}Br, ^{85m}Kr, ^{85}Kr, ^{87}Kr, ^{88}Kr, ^{89}Kr, ^{90}Kr, ^{88}Rb, ^{89}Rb, ^{90}Rb, ^{131}I, ^{132}I, ^{133}I, ^{134}I, ^{135}I, ^{131m}Xe, ^{133}Xe, ^{135m}Xe, ^{135}Xe, ^{138}Xe, ^{134}Cs, ^{137}Cs, ^{138}Cs, ^{139}Cs) and stable (^{83}Kr, ^{84}Kr, ^{86}Kr, ^{131}Xe,^{132}Xe, ^{134}Xe, ^{136}Xe) isotopes.

In the case of leakage during normal operation it is supposed that the free volume of the high temperature fuel rod contains no liquid water but a mixture of gases and steam. Leaking fuel rods continuously release fission products, the intensity of release is characterised by the leakage rate. The free volume of the fuel rods is simulated as a single volume and all isotopes are released at the same rate.

After reactor shutdown the temperature of the fuel elements decreases, the steam inside the cladding condenses and coolant enters the free volume. The conditions inside the cool but still high-pressure fuel element are determined by the gas laws together with the condensation of the steam. There are two phases in the fuel element: a gas phase in the upper part and water in the lower part of the rod. The upper gas volume contains non-condensable gases (He, Xe, Kr, H), while the lower water volume contains volatile fission products (Cs, I, Br, Rb) and dissolved gases (He, Xe, Kr, H). The activity release during transients is driven by the gas volume expansion and the composition of release isotopes depends on the defect location.

During long-term storage in the spent fuel pool the isotopic content will change in the free volume of the fuel rod. Due to the low temperature the fuel rod will be filled by water and the gases will accumulate in the upper part of the rod. Beyond radioactive decay, leakage to the spent fuel pool and the dissolution of fission products from the pellets into the water volume of the fuel rod are the governing mechanisms.

2.11.3 Interlinkage to other codes in radiological consequences evaluation method

1) The TSKGO code uses the isotope release data calculated by the fuel behaviour code FUROM (FUel ROd Model) code, which calculates the release to the free volume of both stable and radioactive gaseous and volatile fission products. The FUROM code provides for each time step the release of each isotope from the pellets into the free volume and the main geometrical characteristics of the rod (e.g. gas volume). The actual amount of the given isotope inside of the leaking rod is calculated by the TSKGO program taking into account radioactive decay and leakage to the primary circuit. The output of TSKGO provides the isotope specific activity release from the fuel rod.

2) The TSKGO calculations needs additional input data (e.g. location and size of defect) which could be provided by other codes or taken from NPP experience. For safety analyses (e.g. SGTR) the boundary conditions could be prescribed by system codes.

3) The main boundary conditions includes the history of primary pressure and reactor power during the transient process (e.g. SGTR). For the simulation of leaking fuel rods in the spent fuel pool additional data are needed on the water level in the pool and on the position of the assembly.

2.11.4 Further development needs

The hydrogen uptake model of E110 alloy will be updated on the basis of new experimental data.

2.11.5 References

[1] Szabó, P., Hózer, Z., Kulacsy, K., Somfai, B., Nagy, R., Burján, T., Baracska Varjú, I., Pintér, T., 2016. Numerical simulation of the telescope sipping of a leaking VVER fuel assembly, Annals of Nuclear Energy, Vol. 99, pp. 345-352

2.12 RING

2.12.1 General overview of the code and modelling capabilities

The RING (Release of Iodine and Noble Gases) code has been developed for the simulation of leaking fuel rods under steady state and transient conditions and the specific parameters of the model for a VVER-440 type NPP have been determined. The steady state model can be applied for the calculation of leaking fuel characteristics using measured iodine and noble gas activity concentration data to predict the number of leaking fuel rods and the amount of tramp uranium during single cycles and during several years of operation. The transient model is capable of predicting the ^{131}I activity peak during operational transients. The RING code is part of the on-line monitoring system of the Paks NPP in Hungary.

2.12.2 Fission product (FP) release and FP transport modelling in the code

The steady state model simulates the release path of iodine and noble gas isotopes from their place of birth in the fuel pellet into the coolant and takes into account the fissions in the tramp uranium on the fuel rod surfaces. The transport of isotopes is driven by diffusion mechanism in the pellet, other release mechanisms (recoil, knockout) are considered negligible. The release from the gap into the coolant is proportional to the inventory of the given isotope in the coolant. The half life periods of the considered isotopes are short enough to reach equilibrium concentrations. Isotopes produced as results of fission in the tramp uranium are promptly released into the coolant. The model applies only to core average characteristics and for this reason gives no information on the burnup and power of the leaking fuel rod or the position of the failure. The following isotopes are taken into account: ^{131}I, ^{132}I, ^{133}I, ^{134}I,^{135}I, ^{85m}Kr, ^{87}Kr, ^{88}Kr, ^{133}Xe, ^{133m}Xe, ^{135}Xe, ^{135m}Xe, ^{138}Xe.

In the transient model the following basic release mechanisms are considered:

- At high fuel pellet temperature the gap is filled by steam and the release of radioactive isotopes is driven by a diffusion mechanism.
- At low fuel pellet temperature the gap is filled by water and a convection type inflow-outflow mechanism drives the release of radioactive isotopes.

The transition between the above two cases is expected at low power, in the present model this limit is set to 100 MW core power. It means that the second leaching mechanism takes place only in the decay power range. In the transient model the release accelerates as a function of changes in primary pressure, core power and boric acid concentration. The release acceleration parameters were determined on the basis of Paks NPP pressure, power and boric acid histories during shutdown for refuelling period with leaking fuel rods.

2.12.3 Interlinkage to other codes in radiological consequences evaluation method

1) First the code calculates the steady state parameters in the reactor with leaking fuel rods and tramp uranium. in the second phase transient calculations are carried out and the primary coolant activity concentrations are predicted.

2) The RING calculations can be carried out using NPP measured data. However, for safety analyses (e.g. SGTR) the boundary conditions could be prescribed by system codes.

3) The main boundary conditions includes the history of primary pressure, reactor power and boric acid concentration during the transient process (e.g. SGTR).

2.12.4 Further development needs

The transient model will be updated in the framework of the EU R2CA project using new shutdown iodine spiking data from a VVER reactor.

2.12.5 References

[1] Hózer, Z. 2014. Simulation of leaking fuel rods in a VVER reactor, Annals of Nuclear Energy, Vol. 70, pp. 122–129

2.13 AC²

2.13.1 General overview of the code and modelling capabilities

The AC² integral code system integrates the thermal hydraulics codes ATHLET, the severe accident code ATHLET-CD and the containment code COCOSYS. AC² and all three codes are developed by GRS, which is the main technical support organization of the German government on nuclear safety. The code system is applied for the analysis of nuclear reactors at normal operation, anticipated operational occurrences and design basis accidents up to severe accident conditions with radionuclide releases from the containment. One main objective of this code system is to provide a state-of-the-art tool for the integral simulation of plant behaviour that can explicitly consider the interaction between cooling circuit and containment [1].

The current release AC² 2019 consists of three main programs:

- ATHLET 3.2 [2] for the detailed thermal hydraulic simulation of the reactor coolant system and spent fuel pool up to design extension conditions without core degradation
- ATHLET-CD 3.2 [3] a plug-in extension of ATHLET for the simulation of design extension conditions with core degradation and severe accidents,
- COCOSYS 3.0 [4, 5] for the thermal hydraulic simulation of containment and buildings from operational conditions up to severe accidents with off-site release.

The main AC² driver controls coupled analyses of ATHLET and ATHLET-CD with COCOSYS (Figure 2.7). Further programs, tools and libraries are included in the program package, e.g. the ATLAS GUI for results visualization.

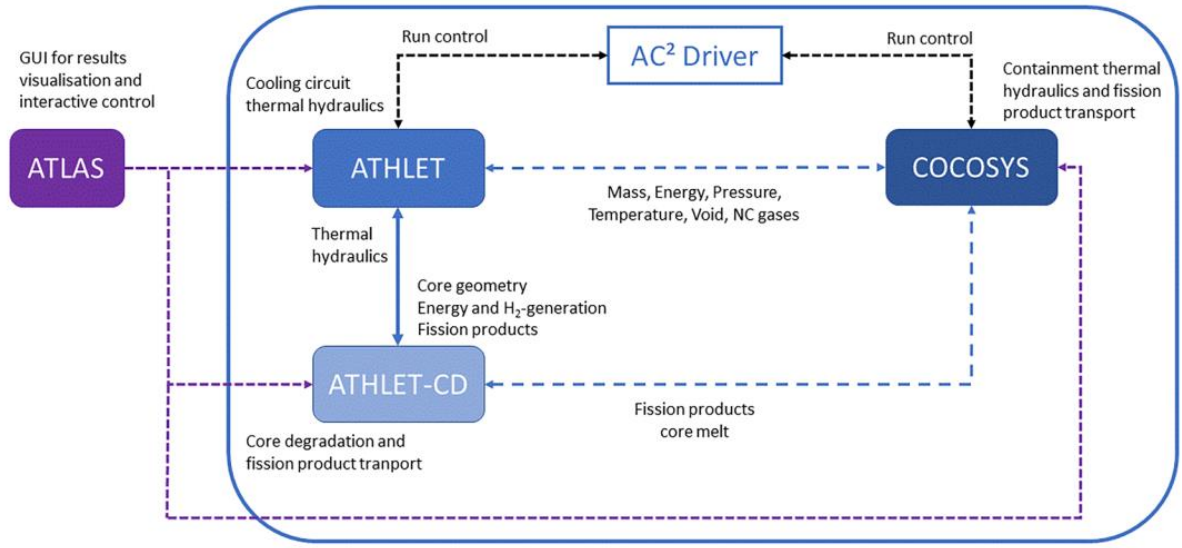

Figure 2.7. AC² architecture [6].

2.13.1.1 ATHLET

The thermal-hydraulic computer code ATHLET (Analysis of THermal-hydraulics of LEaks and Transients) is being developed for the analysis of operational conditions, abnormal transients and all kinds of leaks and breaks in nuclear power plants. The aim of the code development is to cover the whole spectrum of design basis and beyond design basis accidents (without core degradation) for PWRs (including VVER), BWRs, SMRs and future Gen IV reactors with one single code [2].

ATHLET is based on a modular structure to model different physical phenomena. The basic modules of the code are:

- Thermo-Fluiddynamics (TFD)
- Heat Conduction and Heat Transfer (HECU)
- Neutron Kinetics (NEUKIN)
- Control and Balance of Plant (GCSM)

These modules are described below.

In ATHLET development, a strict separation between physical models and numerical methods is applied. The TFD system of ordinary differential equations is solved fully implicitly with the numerical integration method FEBE (Forward Euler – Backward Euler). Other independent modules (e.g. large models with own time advancement procedure) can be coupled without structural changes in ATHLET by means of dedicated interfaces.

TFD module

The TFD module solves the mass, energy and momentum balance for a thermal-hydraulic system, which is described by basic fluiddynamic elements, called thermo-fluiddynamic objects (TFOs). There are several TFO types, which are classified into three basic categories:

- Pipe objects, which employ a one-dimensional TFD-Model describing the transport of fluid. After nodalization according to input data, a pipe object can be understood as a number of consecutive nodes (control volumes) connected by flow paths (junctions).
- Branch objects, which consist of only one control volume. They employ a zero-dimensional TFD model of non-linear ordinary differential equations or algebraic equations.
- Special objects, which are used for network components that exhibit a complex geometry, e.g. the cross connection of pipe objects aligned in parallel for the generation of a multidimensional network.

ATHLET offers two sets of conservation equations. In the two-fluid model with six equations, mass, energy and momentum balance are solved separately for the liquid and vapour phase. In the 5-equation model, mass and energy balance are solved separately for both phases, while a mixture momentum balance with a drift-flux model is applied. Both models can simulate thermal and mechanical non-equilibrium and allow for the presence of non-condensable gases. A 3D model allows explicit consideration of 3D terms in the momentum equations to investigated 3D flow phenomena.

The spatial discretization is performed based on a finite-volume staggered-grid approach. The mass and energy equations are solved within control volumes, and the momentum equations are solved over junctions connecting the centers of the control volumes. The solution variables are the pressure, vapour temperature, liquid temperature and vapour mass quality within a control volume, as well as the mass flow rate (5-eq. model) or the phase mass velocities (6-eq. model) in a junction, respectively.

ATHLET offers the modelling of mixture levels with dynamic sub-division of control volumes into two regions: steam with water droplets above mixture level and liquid with vapour bubbles below mixture level (available for 5-eq. model). A full-range drift-flux model is applied for the calculation of the relative velocity between the fluid phases. The model comprises all flow patterns from homogeneous to separated flow occurring in vertical and horizontal two-phase flow. It also takes into account countercurrent flow limitations in different geometries. ATHLET can model different types of non-condensables (nitrogen, oxygen, hydrogen, air) and a boron tracking model is available. More details of the models are given in [7].

Of particular importance for the current project is the modelling of critical flow, which occurs at the leak (in case of LOCAs) or at the ruptured SG tube (in case of a SGTR event). Critical flow rates are calculated by a one-dimensional thermal non-equilibrium model (CDR1D model) with consideration of the given flow geometry [8, 9]. The model comprises a large range of thermal-hydraulic conditions from strong subcooled of liquid to strong

superheated conditions. Alternatively, a homogeneous equilibrium model and the Moody discharge model are available.

HECU module
The HECU module solves a one-dimensional discretized heat transfer equation for solid structures. Basic geometries like plates or cylinders are considered and there are specific models for, e.g., fuel rods as well. For heat transfer at surfaces, the module considers single- and two-phase flow conditions including critical heat flux, minimum film boiling, quench front progression, evaporation and condensation. Specific correlations for different working fluids can be selected. HECU can also simulate two-dimensional heat conduction in selected structural components.

NEUKIN module
The NEUKIN model offers capabilities for simulation of nuclear heat generation. Two models are available: point-kinetics (one group of prompt and six groups of delayed neutrons) and one-dimensional kinetics model (time dependent neutron diffusion equation with two energy groups of prompt neutrons and six groups of delayed neutrons). The reactivity feedback effects for fuel temperature, moderator density and moderator temperature are calculated either by means of dependencies given by input tables or with reference reactivity coefficients. If the boron-tracking model is applied, the reactivity feedback due to changes in the boron concentration will be also taken into account.

NEUKIN also offers a general interface for coupling of 3D neutronic models, such as coupling to DYN3D [10], which is also applied in the R2CA-project (see Section 2.5).

GCSM module
The simulation of balance-of-plants systems within ATHLET is performed by the basic module GCSM (General Control Simulation Module), which is a block-oriented simulation language for the description of control, protection and auxiliary systems.

Modules for special components
Specific models are provided for the simulation of valves, pumps, accumulators, steam separators, steam and gas turbines, compressors, steam condensers, single and double ended breaks, fills, leaks, and boundary conditions for pressure and enthalpy. The steam separator model is an empirical approach for the calculation of carry-over and carry-under flows by means of input functions of the inlet mass flow rates, of the void fraction in the separator region, and of the mixture level outside the separator. Abnormal separator conditions like flow reversal or flooding can be simulated. In general, major plant components (e.g. pressurizer, steam generators) can be modelled by connecting thermo-fluiddynamic objects (TFOs) and heat conduction objects (HCOs) via input data. Simplified compact models for those components are also available as special objects.

2.13.1.2 ATHLET-CD
ATHLET-CD [3] is a predefined plug-in for ATHLET. ATHLET-CD extends the underlying ATHLET models and inputs with additional modules for the simulation of severe accident phenomena and processes. The most important modules of ATHLET-CD are the described in this section.

ECORE module (core degradation module)
The module ECORE consists of models for fuel rod, absorber rods (AIC or B_4C) and fuel assembly including BWR-canister and absorber. ECORE calculates the core heat-up, oxidation effects and core degradation phenomena. Thereby, the core is described by radial core sections with data blocks for each radial core section in the input file. The fuel and control rods are modelled by one representative fuel and control rod per section. The implemented models consider the following phenomena [11].

- Heating-up of the fuel rods due to release of decay heat,
- Gap heat transfer
- Heat transfer to fluid and heat transfer by radiation
- Mechanical fuel rod behaviour (ballooning and failure of the cladding),

- Oxidation of zirconium and boron carbide,
- Melting, freezing, re-melting and re-freezing of metallic and ceramic components,
- Formation and dissolution of blockages.
- Relocation of molten core material by a candling model [12]

Criterion for cladding failure is selected by the user via input from four options: (1) maximum strain (38%), (2) stress criteria as function of heat-up rate (correlation of Chapman), (3) model of Hagrman, and (4) extended model based on TESPA-ROD.

Quench front model (QUENCHCORE module)
Of particular importance within the project is an appropriate description of the cooling process of the hot fuel rods during the reflood phase of a LOCA accident. During that process, the heat transfer regime changes from film boiling to nucleate boiling. For that purpose, two approaches are available in ATHLET-CD [11]:
The so-called 'spontaneous' rewetting model simulates the rewetting process individually for each single heat conduction volume (sub-division of the modelled rods), taking into account local criteria like surface temperature, heat flux, and fluid conditions in the coupled fluid CV. It follows the HTC scheme described in the ATHLET documentation [7]. This model is applicable mainly for high-pressure conditions, e.g. for early rewetting during the blowdown phase of a LBLOCA.

During the refill and reflood phase of a LOCA, however, steep axial temperature gradients may occur along the fuel rods and internals in the vicinity of the quench front, which require the axial heat conduction to be considered. Furthermore, high local heat fluxes, which occur during rewetting, would require an expensive fine mesh nodalization of the rod. In this case, the use of the quench front model is recommended (Figure 2.8). The calculation of upper and lower quench front positions by means of analytical correlations takes into account axial heat conduction in the cladding as well as pre-cooling of the dry rod surface near the quench front, and reduces the influence of nodalization on the calculated results.

The upper quench front is particularly important for Siemens-KWU type PWRs (German design) with combined ECCS injection (injection from cold leg and from hot leg).

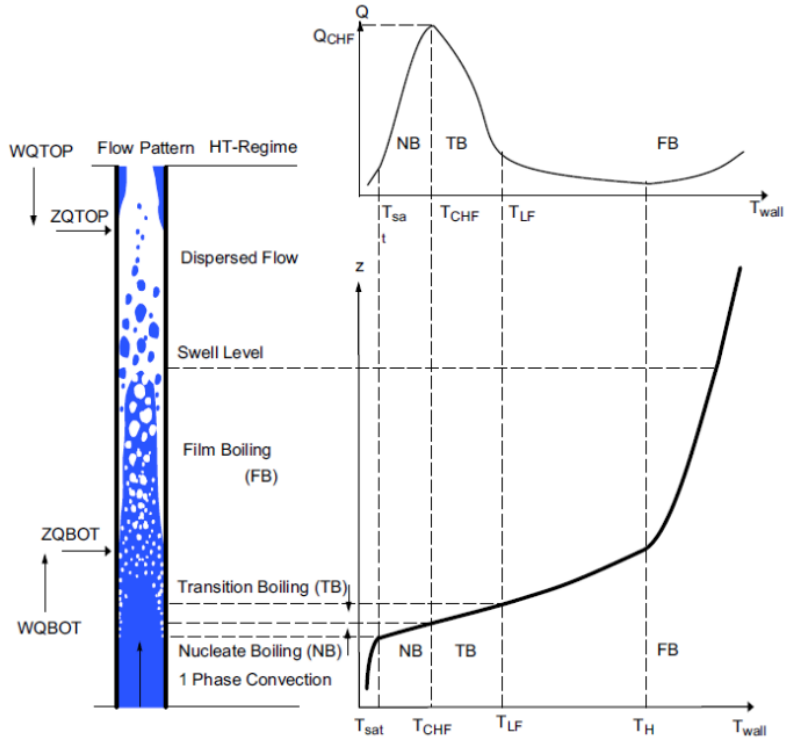

Figure 2.8. Correspondence between flow pattern with quench front model data and heat transfer regimes [11].

The Semeria/Martinet correlation [13] is applied for calculation of the lower quench front velocity (WQBOT):

$$w_{\mathrm{Q,bot}} = \frac{1}{\rho_{\mathrm{c}} c_{\mathrm{c}}} \sqrt{\mathrm{HTC_Q} \frac{\lambda_{\mathrm{c}}}{\delta_{\mathrm{c}}} \frac{T_{\mathrm{LF}} - T_{\mathrm{sat}}}{\sqrt{(T_{\mathrm{H}} - T_{\mathrm{sat}})(T_{\mathrm{H}} - T_{\mathrm{LF}})}}} \quad (1)$$

The Yamanouchi correlation [14] is applied for the calculation of the upper quench front velocity (WQTOP):

$$w_{\mathrm{Q,top}} = \frac{1}{\rho_{\mathrm{c}} c_{\mathrm{c}}} \sqrt{\mathrm{HTC_Q} \frac{\lambda_{\mathrm{c}}}{\delta_{\mathrm{c}}} \frac{T_{\mathrm{LF}} - T_{\mathrm{sat}}}{T_{\mathrm{H}} - T_{\mathrm{LF}}}} \quad (2)$$

With velocity of quenchfront w_{Q}, cladding density ρ_{c}, cladding heat conductivity λ_{c}, cladding heat capacity c_{c}, cladding thickness δ_{c}, Leidenfrost temperature T_{LF}, saturation temperature at the quench front T_{sat}, cladding temperature on the hot, unrewetted side of the quenchfront T_{H}, and the heat transfer coefficient at the quenchfront $\mathrm{HTC_Q}$. More details are given in [11].

OREST module

This module contains the stationary part of the nuclide program system of ATHLET-CD and calculates the nuclide inventory in the fuel rods for light-water reactors. The one-dimensional space-cell burn-up program has been part of ATHLET-CD since version 2.2A and is based on an earlier GRS development [15].

OREST calculates the nuclide inventory in fuel rods in an automated HAMMER-ORIGEN system [15]. The calculations can be performed in square or hexagonal grids for different fuels. In addition to the known ORIGEN [16] results, the development of the neutron spectra, the multiplication factor, the rod temperatures, the fission product poisoning, the effective energy per fission, the macroscopic capture and fission cross sections and the neutrons per fission are calculated.

The material composition of nuclear fuel changes as the fuel assemblies are depleted. This change has considerable effects on the nuclear cross sections, since both the macroscopic neutron spectra (i.e. hardening) and the microscopic cross sections (of e.g. U-236, U-238, Pu-240, Pu-242 as important isotopes) change. An exact burn-up calculation must therefore take these changes in the course of the burn-up into account. This is achieved in OREST by coupling of ORIGEN with the fuel grid program HAMMER. For this purpose, ORIGEN is supplied after certain burn-up periods with nuclear cross sections, which are re-determined in the current fuel mixture from current flux and cross section calculations by HAMMER.

HAMMER calculates the neutron flux and the effective cross-sections for 84 energy groups (30 groups of thermal neutrons and 54 groups of epithermal and fast neutrons). The superordinate OREST transforms these values to the three energy groups required in ORIGEN (thermal neutrons up to 0.5 eV, resonance range and fast neutrons above 1 MeV). The calculation of the nuclide data is based on the nuclide database ENDF/B-V [17].

The user can define the fuel type (fuel assembly grid type, pellet and cladding geometry, cladding material, coolant/moderator material, and enrichment), the power history and the boron concentration in the ATHLET-CD input deck. OREST performs the burnup calculation for the fuel with given time steps and generates tabular values. This data is used by the FIPISO module as initial values for the transient calculation (see next subsection). More details about OREST are given in [15, 18].

FIPISO module

This module contains the transient part of the nuclide code package. It calculates the masses, power and activities of the core material and of the released masses during a transient. FIPISO describes the behaviour of the elements and isotopes in the entire primary circuit (up to 1296 nuclides). The module is based on stand-alone code FIPISO-98 developed by GRS [18, 19].

FIPREM module

FIPREM calculates the fission product (FP) release from the fuel rods after cladding failure. It is described in Section 3.13.2.2.

Fission product and aerosol transport module SAFT
The transport and deposition of radionuclides in the primary coolant system can be simulated by the module SAFT which is based on SOPHAEROS V2 which is be developed by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) in France. Its main features are described in Section 2.13.2.2.

2.13.1.3 COCOSYS

COCOSYS (the COntainment COde SYStem) is a lumped parameter computer code developed and maintained at Gesellschaft für Reaktorsicherheit (GRS mbH) and used for best-estimate analysis of light-water reactor containments during severe accidents. Code assignment is to simulate all relevant phenomena, processes and conditions inside the containment that may occur during severe accidents (it should be noted that code is also able to simulate design basis accidents). One focus of the COCOSYS is on the extensive consideration of interactions between the various developing phenomena, such as the thermal hydraulics processes, hydrogen combustion, and aerosol and nuclide behaviour.

The structure of the COCOSYS is shown in Figure 2.9 [5]. Each of the main modules is a separately executable program, dedicated to one specific area of the overall problem. Communication among these main modules is effected via MPI (the message passing interface library) or PVM (parallel virtual machine). The main driver organises and controls the calculation sequence, the individual main modules calculate the overall problem in such a way that they can be coupled at a time-step level, that is the extent of the parameters to be exchanged is relatively low. Apart from the three main modules THY, AFP and CCI that belong to the inner part of the COCOSYS system, further programs are also coupled to the COCOSYS, namely the LAVA code (GRS) for the simulation of the spreading and dislocation of the melt. As regards the coupling, the overall concept in the COCOSYS is implemented in such a way that different modules can run in parallel. The results (output data) can be visualised both online and offline with the ATLAS program [5, 20].

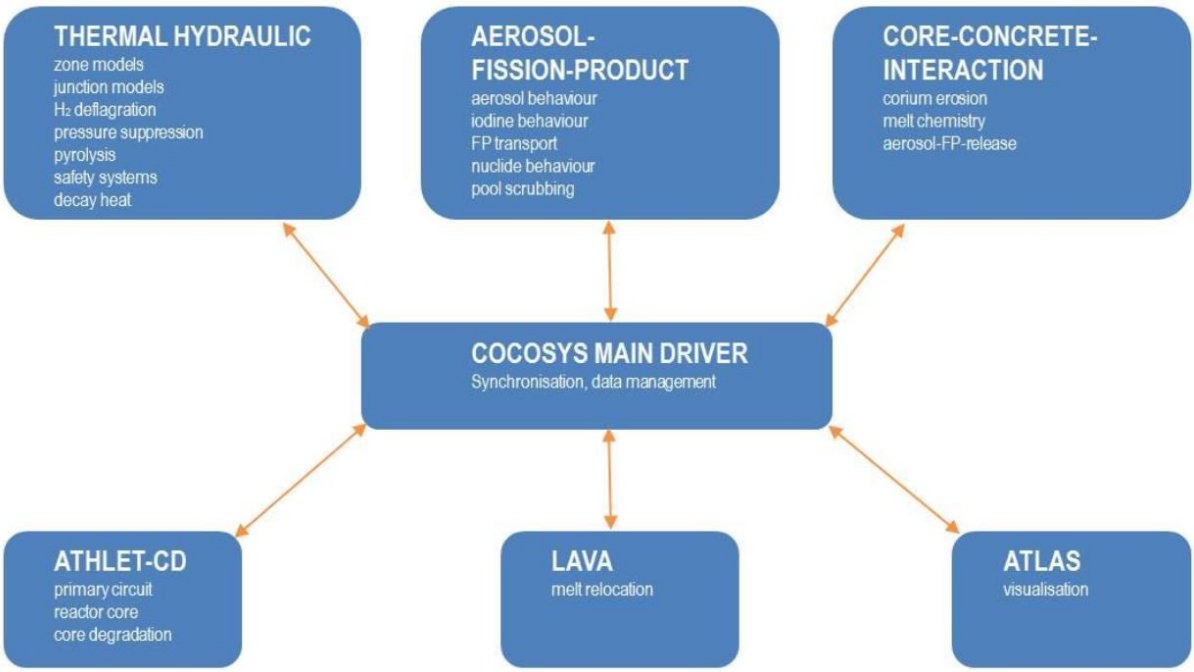

Figure 2.9. Structure of COCOSYS.

The COCOSYS code consists of the following main modules [5]:

- THY – thermal hydraulic;
- AFP – aerosol-fission-product;

- CCI – core concrete interaction.

The LAVA special application, which is a part of the COCOSYS system, is used for the melt spreading modelling.

THY module

THY module feature is that the compartments of the considered power plant or other building types have to be subdivided into control volumes (zones); each zone can be split into several so-called zone parts. The thermodynamic state of a zone is defined by its temperature and masses of the specified components.

Six different zone models are implemented in the COCOSYS:

- equilibrium zone model;
- non-equilibrium zone model;
- hydrogen burning zone model (DECOR);
- pressure suppression zone model (DRASYS);
- jet vortex condenser model (VORTEX);
- interface zone model.

In equilibrium zone model all components (liquid water, vapour and other non-condensable gases) are assumed to be mixed homogeneously, resulting in a homogeneous distributed temperature in the control volume. Superheated as well as saturated conditions are considered, herewith superheated atmospheres cannot contain liquid water - in these cases the water is drained immediately into other zones.

In non-equilibrium model, the zone is subdivided into two parts: the atmosphere part similar to the equilibrium zone model and a sump part (if exists) specified by the temperature and water mass. Heat and mass exchange between these two parts is possible and is simulated by convection and condensation (or evaporation) correlations. In case of a coupled THY-AFP simulation the deposition rates of fog droplets are based on the AFP calculation.

Hydrogen burning model is based on the equilibrium zone model as equations describing on the thermodynamic gradient of the control volume. DECOR combustion model is a one dimensional, but three burning axes can be defined for flame progression within a coordinate system towards the containment. During a deflagration process the zone is subdivided into an unburned and a burned zone part. The propagation of the flame results in a calculated burning velocity and a gas expansion behind the flame. Also the COMB/FRONT model exists – this is a simplified alternative model to simulate hydrogen combustion and flame front propagation.

In the DRASYS pressure suppression model the zone is subdivided into three zone parts: the pipe, the atmospheric part above the pool and the water pool zone part. DRASYS is able to simulate the dynamic pressure behaviour resulting from the dynamics of the water level in the pipe, the content of bubbles and condensation processes at the bubbles surface.

Jet vortex condenser (JVC) model is designed for the description of dynamic processes in a jet vortex condenser installed at NPPs with VVER-440 Model 230. A VORTEX zone is subdivided into four zone parts: downcomer or the gas volume above the water, vortex chamber or the gas volume behind the water including the gas volume of recirculation tank, water pool and water in the recirculation tank, if the water is present there. The equilibrium zone model equations determine the thermodynamic state of the zone parts. The VORTEX model takes into account the following aspects of phenomenology of an accident with large mass and energy release into the confinement: JVC water is pushed from the downcomer through the jet nozzles into the vortex chamber; going on flow swirling and level increase in the vortex chamber whereas the water level in the downcomer simultaneously decreases; when the water level at the periphery of the vortex chamber reaches its upper edge, the water starts to flood the recirculation tank and flows through recirculation pipes back into the pool inside the vortex chamber; non-condensable gases are directed via the outlet corridor to the environment.

Interface zone model can be used for the coupling of the COCOSYS with a CFD code (such as CFX). The needed thermodynamic state variables (for some selected control volumes or zone parts of this volumes) are delivered by the connected CFD code.

The COCOSYS system includes also inherent additional models to describe the relationship between zones models and modelling of safety systems: junctions, structure objects, special safety systems.

Junction models describe the flow interaction between different volume zones. The simulation of the gas flow and water drainage is strongly separated, although water can be transported via atmospheric junctions by the gas flow and dissolved gases can be transported via drain junctions. Specific junction models are also implemented, like rupture discs, atmospheric valves, flaps/doors, pressure relief valves. Several models are realised for simulation of the water drainage, describing the sump balance, water flow through pipes and along walls. The pump system model is flexible enough to simulate complete cooling systems (e.g. emergency core cooling systems).
Structure objects represent the walls, floors and ceilings of the containment building (all types of metallic and non-metallic heat structures within zones and between them). The heat flux calculation is one-dimensional. Two types of geometry are allowed: plate-type and cylindrical structures, both types of the structures can be divided into layers. Gaps inside a structure are possible as well. The heat exchange between structures and their assigned zones is calculated via convection, condensation or radiation (including wall-to-wall) heat transfer correlations.

THY main module includes models for simulating the safety systems, such as different types of coolers (include atmosphere cooling system), spray systems, ventilation systems, ice condensers and catalytic recombiners. A special one-dimensional model was developed for passive autocatalytic recombiners, using diffusion equations for the reaction on the catalytic surface (include CO recombination).

It should be noted that THY module was extended to include the simulation of oil and cable fires [5].

AFP module
The aerosol-fission-product main module is used for best-estimate simulations of the fission product behaviour in the containment of LWRs. Both the THY and the AFP main modules consider the interactions between the thermal hydraulics and aerosol fission product behaviour. It should be noted that there is a distinction in the COCOSYS in the simulation of aerosol particles, radioactive fission products and the iodine chemistry, i.e. they are simulated by different modules: AERIKA, FIPHOST, FIPISO, AIM and SPARC.

The AERIKA module is responsible for modelling aerosols. It calculates behaviour of up to eight different aerosol components with account for the thermal hydraulic boundary conditions. The module differentiates between soluble and insoluble as well as hygroscopic and non-hygroscopic aerosols. The following deposition processes are covered: sedimentation, diffusive deposition, thermophoresis and diffusiophoresis. For the calculation of the condensation on the aerosols, the moving-grid method MGA is applied, which reduces the numeric diffusion.

The FIPHOST module calculates the transport of the fission products within the containment. The fission products are treated as the radioactive part of the aerosol particles and the radioactive non-condensable gases, whereas their mass is not considered in the model. The fission products can be deposited on surfaces in the atmosphere and in the sump. All relevant processes relating to the fission products are considered: deposition of aerosol particles by natural processes or aided by technical systems such as filters and spray systems, washing-off from walls, and carrier change due to radioactive decay.

The FIPISO module simulates nuclide behaviour considering the reactor's initial core inventory (pre-calculated by other codes) and calculates on this basis the decay of the fission products according to the time of the onset of the release by using established nuclide libraries (analogous to ORIGEN). The decay energy in the individual zones is taken into account in the THY main module. The FIPHOST and FIPISO modules are considering between 400 and 600 different nuclides.

The AIM module simulates near 70 iodine different reactions; AIM distinguishes between 17 iodine species in the atmosphere and 11 iodine species in the sump. The behaviour of the aerosol iodine species CsI and iodine oxides is calculated directly by the aerosol model in AFP (AERIKA module).

The SPARC module regard the retention of aerosols during gas transport through water pools, what allows among other things the simulation of «pool scrubbing» in the pressure suppression system of a BWR.

It should be noted that there are special models in COCOSYS for the simulation of filters (HEPA filters, granulate filters) which also consider the increasing pressure loss in the atmospheric junctions (THY module response) [5].

CCI module

The COCOSYS core concrete interaction main module is based on the code MEDICIS, which was originally developed by IRSN and GRS for the integral code ASTEC (now, CCI is further developed in GRS's sole discretion). CCI uses a lumped parameter approach and is based on a layer averaged description of the pool configuration. The pool may be formed by one or two layers plus a crust on top of the upper layer: the top crust can be described using either a simplified (not forming a separate layer) or a detailed model (forming a separate layer). Solution of the mass and energy balance equations is made independently of the detailed corium chemistry evolution. The melt pool may be either homogeneous (1 layer and potential top crust) or stratified (2 layers and potential top crust) and may evolve versus time. Four crust layer types are possible: an oxide layer, a mixed oxide/metal layer in the case of a homogeneous pool, a metallic layer and the upper crust built-up at the pool upper interface (for detailed top crust model).

The cavity geometry is either axisymmetric or is slab-shaped with two non-ablatable walls. The 2D-profile of the cavity boundary versus time is determined using the local energy conservation at each boundary node and the Stefan's relation to evaluate the ablation velocity. Heat transfer between melt and concrete is calculated on the basis of a distribution of effective heat transfer coefficients along the pool interface in combination with a concrete decomposition temperature. The upward heat transfer from the upper interface of the pool to the surrounding is calculated considering radiation and convection processes. A simplified model takes into account the formation of a quasi-steady upper crust under dry conditions. In case of top flooding conditions, CCI equates the heat flux through a potential top crust with the heat flux obtained from the approximated boiling curve. The configuration of the pool may be static or dynamic; the criterion in the dynamic configuration model for switching between a mixed or a stratified configuration depends on the gas bubbling in the melt.

A consistent set of simplified enthalpy functions is used for all species either in the condensed phase or in the gaseous phase permitting to take into account oxidation reactions; an additive law is used for evaluating the heat capacity of mixtures. Under top flooding conditions a boiling model is available that calculates the heat flux through the top interface of the corium pool including a developing crust layer under consideration of a Nukiyama boiling diagram. The CCI fission product release model takes into account the process of vaporisation of species by assuming a thermodynamic equilibrium of the melt in contact with a gaseous phase and is based on methods provided in ASTEC's ELSA module [5].

LAVA special application

The code LAVA was developed as a model for the simulation of core melt behaviour to be used as part of the COCOSYS system. LAVA focusses on the spreading of a viscous melt (or Bingham plastic) driven by the force of gravity; in this approach in the view of a force balance, LAVA assumes a balance of viscous forces and gravity, i.e. inertial forces are neglected. Thus the application of LAVA is restricted to cases in which a melt spreads at small inlet mass fluxes with a significant viscosity or yield stress. Because of that, LAVA is currently provided as a standalone tool within the COCOSYS package, that allows to analyse a certain spreading process in offline mode in relation to COCOSYS simulations.

The basic idea followed with LAVA is the analogy of core melt spreading to volcanic lava flows. Here, because of the very low aspect ratio, the transport of the melt is approximated by a quasi-stationary solution of the lubrication equations – the melt distribution on a 2D-plane is expressed by the melt layer's thickness. The cross section through the melt layer at each location is assumed to be isothermal for the calculation of the velocity profile with constant rheological material properties (viscosity, yield stress). Since the thermal boundary layers in a film flow of oxide melts are very small, the approximation of velocity profiles with constant viscosity throughout the melt thickness at one location is reasonable. For superheated liquids the Newtonian stress-strain-relationship is applied.

The pressure field is assumed to be hydrostatic; the equation of continuity is solved in its depth-integrated version by an explicit algorithm. Though the Navier-Stokes equations are reduced to a one-dimensional formulation, spreading of the melt on a two-dimensional surface is simulated by the application of a cellular automaton method. Heat losses by radiation from the free surface and by conduction into the substratum are taken into account. Crust growth is considered at the free surface, if the surface temperature of the fluid falls below the crust formation temperature between the liquid (or mushy) melt and the solid crust [5].

Coupled calculations with ATHLET-CD

The COCOSYS coupled calculation with ATHLET-CD is necessary in case of a relevant feedback of the containment behaviour to the behaviour inside the primary circuit. The coupled calculations COCOSYS/ATHLET-CD consist in the interconnection of the following processes and phenomena: break flow, primary system heat losses, pump systems interfaces, aerosol and fission product release.

Regarding to the break flow for each discharge object defined in the ATHLET-CD input file the mass and energy flow rate will be transferred to the COCOSYS driver; the possible components are: liquid water, vapour, nitrogen, oxygen, hydrogen, air and carbon dioxide. The heat losses from the primary systems simulated with ATHLET-CD may be directed into the containment simulated with COCOSYS; each heat conducting object in ATHLET can be assigned to one COCOSYS zone. Pump systems interface concept lies in distinguishes between break flow and flow rates at pump system branches; the reasons are that these branches may be connected to spray systems for example and there may be a redistribution of fission products and iodine species on the containment side. Aerosol and fission product release into containment simulated with COCOSYS can be considered using the core degradation part in ATHLET-CD; in the first step the isotope sources are rescaled according to the element release calculated by SOPHAEROS, in the next step the release of chemical components, which are directly assigned to an aerosol species is calculated; in case the FIPISO module is used on the ATHLET-CD side, the compressed nuclide library created by ATHLET-CD is used in COCOSYS also [5].

Calculation boundary conditions for CFD-code

In the COCOSYS program system a part (or the whole) of control volume(s) can be simulated with the CFX code. For the same volume the THY main module has to use the INTERFACE zone model; this model calculates further thermal hydraulic values for other models or for main modules (like AFP) [5].

Keep in mind that the couplings to CFX (ANSYS CFD code), DET3D (CFD tool for simulating H_2 combustion in NPP safety) and LAVA special application are not fully completed and are in a somehow developing status [5].

Export of COCOSYS resulting data

Using COCOSYS it is possible to export different type of data [5]:

- creation of a formatted or unformatted output file with a constant structure in parallel to the plot output data;
- export of core inventory data for ASTEC, ASTRID and MELCOR (the use of this option will ensure consistent data for decay heat calculation and fission product inventory since in the mentioned programs the decay of nuclides is not simulated).

The formation of sensitivity parameters

To investigate the influence of model uncertainties on the results it is partially possible to modify parameter or factors of certain models. This possibility exists for the THY and AFP main modules. All possible sensitivity parameters in the THY main module are linked to heat transfer modelling. For the AFP module all available sensitivity parameters are linked to the iodine chemistry model AIM [5].

SUSA (GRS software for uncertainty and sensitivity analysis) can be applied to COCOSYS results: in this respect unformatted *.pd files are used (user defined output option); it should be noted that SUSA cannot directly start COCOSYS (in comparison with e.g. ATHLET-CD) to run the some kind runs – therefore, these runs must be started manually either by the new COCOSYS GUI or with special batch routines [5].

2.13.2 Fission product (FP) release and FP transport modelling in the code

2.13.2.1 ATHLET

The ATHLET code does not contain any capabilities to calculate the release and transport of fission products.

2.13.2.2 ATHLET-CD

Fission product release is simulated by FIPREM module and fission product transport in the primary circuit is simulated by the fission product and aerosol transport module SAFT.

The module describes:

- the release of fission products (Xe, Kr, I, Cs, Rb, Br, Te, Se, Ag, Ba, Sr, Ru, Pm, Sm, Eu, Gd, Nb, Nd, Pr, Pr, Ce, La, Y, Mo, Pd, Tc, Rh, Sb, Zr),
- the release from fuel and actinides (U, Pu, Np, Am, Cm, Bk, Cf, Es),
- the release of material from the control rods (Ag, In, Cd),
- the release of structural materials (Zr, Sn, Fe, Cr, Ni, Mn).

The calculation is based on rate approaches (Arrhenius equations) or for some elements as a function of the partial pressures.

The following options are available in the ATHLET-CD version 3.2 [3, 11]:

- Option 1: Release rates according to ORNL data (NUREG/CR-6261, [21]) and CORSOR data for the release of the absorber materials silver (Ag), indium (In) and cadmium (Cd),
- Option 2: Release rates according to ORNL data (NUREG/CR-6261) and as a function the partial pressures for the release of Ag, In and Cd,
- Option 3: Release rates according to ORNL data (NUREG/CR-6261), and as a function the partial pressures for the release of the absorber materials Ag, In and Cd and the high-volatile fission products xenon (Xe), cesium (Cs), tellurium (Te), silver (Ag), antimony (Sb), the semi-volatile fission-products barium (Ba), strontium (Sr), ruthenium (Ru) and molybdenum (Mo), and the low-volatile elements zirconium (Zr), Uranium (U) and tin (Sn).

The rate equation approach (according to ORNL data) is similar to CORSOR-M approach:

$$r_x = A_x r_0 e^{(-Q/RT)}, \tag{3}$$

with activation energy $Q = 55\text{kcal} \cdot \text{mol}^{-1}$, the universal gas constant $R = 0.001987\ \text{kcal} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$, and the temperature T. The release coefficient (based on noble gas release) $r_0 = 200\ \text{s}^{-1}$. The scaling factors A_x depend on the material and the fuel conditions (burn-up, cladding oxidation, fuel oxidation), and are given in Table 2.2

Table 2.2. Values of the scaling factor A_x in Eq. (3).

Rod condition	Elemental Scaling factors A_x								
	Xe	Kr	Cs	I					
High burn-up	1.0	1.0	1.0	0.8					
Low burn-up	0.5	0.5	0.5	0.4					
	Te	Sb	Sn						
Cladding fully oxidized	0.8	0.5	0.4						
Cladding not fully oxidized	0.2	0.2	0.2						
	Ba	Sr	Eu	Mo	Ce	U	Ru	Mn	Fe
Fuel oxidation UO_{2+x} $x \leq 0$	0.2	0.1	0.1	0.01	$2 \cdot 10^{-3}$	$6 \cdot 10^{-5}$	$4 \cdot 10^{-5}$	0.0	0.0
Fuel oxidation UO_{2+x} $x > 0$	0.02	0.01	$6 \cdot 10^{-5}$	0.25	$2 \cdot 10^{-4}$	$6 \cdot 10^{-4}$	0.02	0.1	0.02
	Zr	Pu							
No change	$2 \cdot 10^{-4}$	$2 \cdot 10^{-5}$							

For Option 2 and Option 3, the release rates of certain elements are calculated by using the partial pressure of the material [22, 23]. The release flow of a particular component x is

$$\frac{dM_x}{dt} = -r_x M_{0,x}, \tag{4}$$

with the mass at the beginning $M_{0,x}$ and the release rate r_x. Integration of Eq. (4) over time τ with constant release rate yields the local release $R_{x,ij}$ in a core mesh ij:

$$R_{x,ij} = 1 - \frac{M_{x,ij}}{M_{0,x,ij}}. \tag{5}$$

Thus, the mass at the end of an integration time step is calculated by:

$$R^k_{x,ij} = M^{k-1}_{x,ij} e^{-r_{x,ij}\Delta t}. \tag{6}$$

Assuming that the release rate of a component is independent of other components and independent of the composition of the melt, but proportional to the ratio between the partial pressure of the component and the system pressure, the release rate of a material x in a core mesh ij amounts to [22]:

$$r_{x,ij} \approx \Gamma_{x,ij} = K_x T^{0.75}_{x,ij} \frac{p_{x,ij}}{p_{g,ij}}, \tag{7}$$

with $\Gamma_{x,ij}$ evaporation rate of component x in the core mesh ij, K_x a material constant, $T_{x,ij}$ the temperature, $p_{x,ij}$ the partial pressure, and $p_{g,ij}$ the system pressure. Thus, the release rate depends on the temperature, the system pressure and the partial pressure.

The correlation between the temperature T and the (saturation) partial pressure p_x of a pure material x can be described by the Antoine equation:

$$\log p_x = A_x - \frac{A_x}{T + C_x}, \tag{8}$$

$$p_x = e^{A_x - B_x/(T+C_x)}, \tag{9}$$

However, this equation with only three parameters is, in general, not able to describe correctly the complete saturation vapour pressure curve, instead of that a definition in sections is necessary. Nevertheless, in consideration of the fact that only a certain temperature range is simulated, the basic form of the equation is used.

The vapour pressure over an alloy is

$$p_{x,\text{alloy}} = \beta_x p_x, \tag{10}$$

with the activity β_x within the alloy. Finally, equations (7), (9) and (10) yield the release rate:

$$r_x = K_x T^{0.75}_{x,ij} \beta_x \frac{1}{p} e^{A_x - B_x/(T+C_x)}, \tag{11}$$

where T is the local temperature and p is the local pressure.

First, this approach was implemented for the absorber materials Ag, Cd, and In (Option 2), where the coefficients of the Antoine equations could be extracted from the literature, see Table 2.3.

Table 2.3. Values of the coefficients in Eq. (8) and (9).

Element	Unit of p	Unit of T	A_x	B_x	C_x	References
Ag	atm	K	5.615	13680	0.0	[24]
Cd	Torr (mm Hg)	K	7.897	5217.8	0.0	[25]
In	atm	K	5.19	12170	0.0	[26]

Some difficulties arose in finding the appropriate constants for the fission products and other structural materials (option 3) [23]. In order to estimate first rough values, data from the tables [27, 28] were evaluated and the coefficients were calculated. To simplify the calculation, $C_x = 0$ was set. Afterwards, the values were compared to results obtained from the Phébus experiments FPT1, FPT2 and FPT3, and the values were optimized in such

way, to obtain the best fit to the experimental results [23]. Unfortunately, the finally applied coefficients are not given in any open report and may be requested directly from the code developer GRS.

The **transport and deposition of radionuclides** in the primary coolant system can be simulated by the module SAFT which is based on SOPHAEROS V2, which is be developed by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) in France. The input of the thermos-fluiddynamic data, the surface temperatures and the release data are given by several ATHLET-CD modules. All the chemical effects and the phenomena during the transport are calculated by SAFT. For that purpose an own material database is used [11].

Possible physical states are [11]:

- Suspended vapour
- Suspended aerosols (condensed vapour and non-volatiles)
- Condensed vapour deposited on circuit walls
- Aerosol deposited on circuit walls (non-volatiles with condensed vapour)
- Vapour of volatiles sorbed in circuit walls

Currently, the following phenomena are implemented [11]:

- Chemical interaction in gas phase
- Coagulation or agglomeration of suspended aerosols
- Deposition of suspended aerosols on circuit walls and re-suspension
- Vapour condensation/evaporation on/off walls and aerosols

Optionally the chemical compounds, which should be considered in the simulation of the circuit, can be selected.

The description of the module SAFT, currently open to the public, is very limited. As the module is based on SOPHAEROS, for further information, the reader is referred to [29, 30].

2.13.2.3 COCOSYS

Fission product release and transport is simulated via AFP module: FP transport is modelled via FIPHOST model, FP release/decay – via FIPISO model. FP release and transport includes the following processes:

- fission products release into containment during a severe accident in a LWR (LOCA e.g.) from the molten core in the cavity or by melt droplets injected during direct containment heating;
- the FP's association with carriers or hosts;
- drainage of the aerosols deposited on wall by down running water films into the containment sumps (taking into account FP's accumulation in filters or their wash out by spray systems);
- resuspension of the FP's deposited on dry surfaces during a H_2 combustion and FP's dissolved in a boiling sump.

In reality FP transport and radioactive decay occur simultaneously. But the changes of the isotope inventory in a compartment of the containment due to FP transport are much faster (characteristic time 1÷10 s) than the changes due to radioactive decay (only long-lived isotopes form the inventory since the short-lived isotopes have already been decayed in the reactor core or on their way through the primary system). Therefore, the FIPHOST can be numerically separated from the decay model FIPISO [5].

Fission product transport

At the moment all relevant FP transfer processes can be simulated within a five-host concept therefore, it was chosen for FIPHOST (three mobile hosts are gas, aerosol and water; two immobile hosts are the gas and water space surfaces). The following general model assumptions have been established for FIPHOST:

- FP's have no mass with respect to thermal hydraulics;
- FP's produce heat, which influences the thermal hydraulics;
- no chemical reactions are considered (chemistry of iodine in AFP part);
- no FP element mass changes by decay are considered.
- no FP vapours which condense on aerosols and surfaces are considered;
- instantaneous host change caused by isotope decay is assumed.

The fission products are associated with non-condensable gases or aerosol components, i.e. they are transported with gases/aerosols or deposited with aerosols. The association of FP's with water (i.e. fog) is not allowed. Corresponding to the five hosts concept the FP's are carried with the mobile hosts and deposited on immobile hosts; additionally, fission products can deposit themselves in recombiners or in filters. The number of FP elements, isotopes and hosts is not limited in FIPHOST. The five fission product hosts in a COCOSYS control volume, the hosts for engineered systems and the removal processes for the hosts are shown schematically in Figure 2.10 [5].

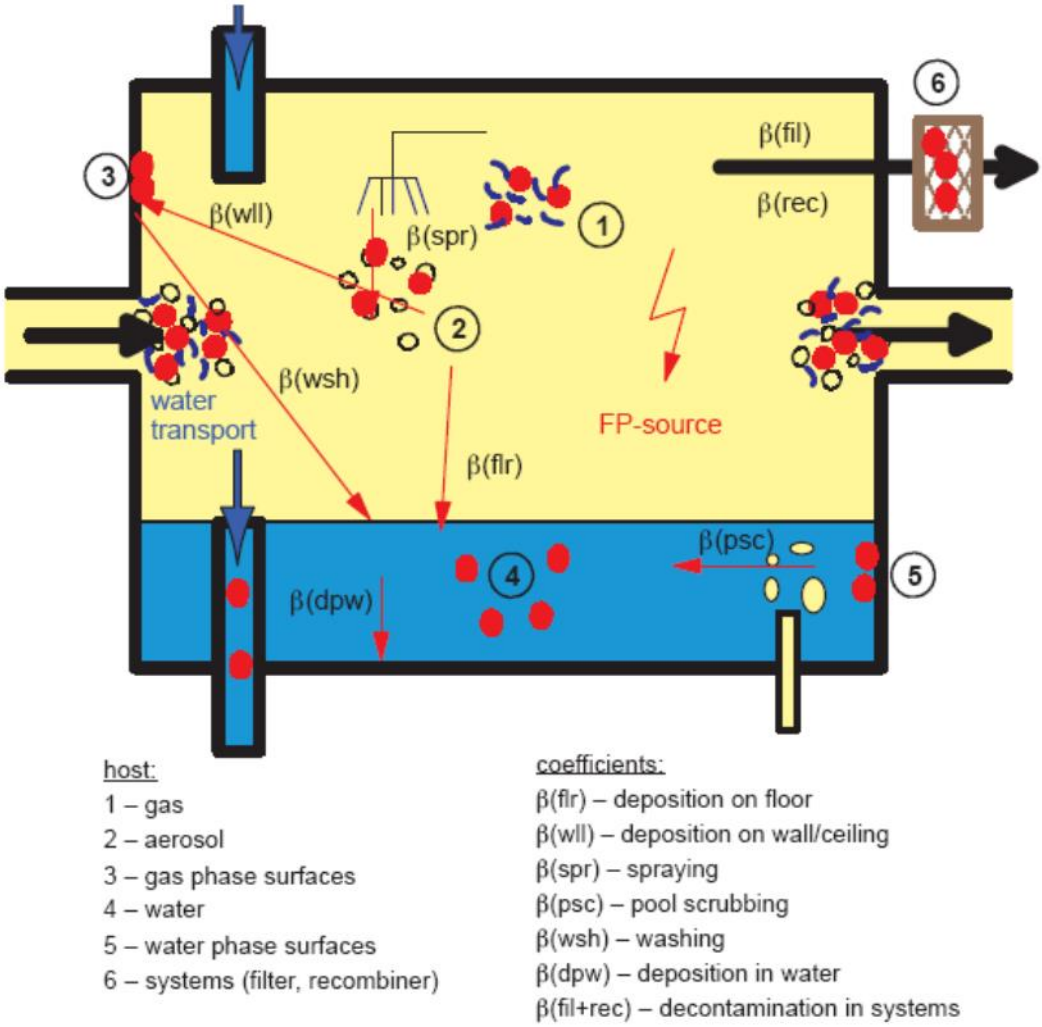

Figure 2.10. FIPHOST control volume, fission product hosts.

The transport of gaseous fission products (host 1) is linked with the volume flow rates through atmospheric type junctions and fan systems. Aerosol type fission products (host 2) behave like the assigned aerosol component (an element can be assigned to just one aerosol). Here it has to be considered, that ceilings and side walls are combined to the «gas surface» (surfaces connected to the atmosphere, host 3). The deposition rate of aerosols onto the floor is used for the fission product deposition into the sump volume (if existing). Fission products suspended in sump volumes (host 4) are transported with the water according the drain and pump flow rates calculated in the THY module. For the fission product deposition in the sump to «water surfaces» (surfaces connected to the sump volume, host 5) an «own» model is used, because suspended aerosols in the sump volume are not simulated. Fission products deposited on «gas surfaces» (host 4) might be washed-down. Fission product deposited on «water surfaces» (host 5) might be resuspended, in case that the sump water volume exchange rate exceeds a user defined limit. The wash-down of FP's is considered via a rate dependence, based on condensation flow rate, wall surface area, water density and film thickness. The wash-out of fission products by spray droplets is considered via a rate dependence, based on the relative change of aerosol mass due to wash-out by spray [5].

Fission product behaviour and sources
Using the FIPISO module the behaviour of all nuclides relevant for the mass transport and heat release in the containment can be simulated (up to 1296 isotopes inside each zone separately). The module considers the core inventory of the reactor at the initial accident time and calculates the decay of the activity and the decay heat release. For the use of the module some additional files are necessary (using the OREST module in ATHLET-CD these files can be calculated): library file containing the nuclide library; compress file containing the compress instructions to reduce the number of isotopes (only relevant isotopes are of interest); inventory file(s) containing the decay data of the core(s).

The FP source can be grouped specifying the FP-profile. Using profile data, it is assumed, that the relative mass fraction is constant within one group [5].

Fission product decay heat
In COCOSYS several concepts to simulate FP's decay heat are implemented:

- use of FIPISO module – the decay heat is calculated on the basis of library data in standalone COCOSYS or in coupled ATHLET-CD/COCOSYS calculations;
- use of input file based on elements;
- use of input file based on ASTEC calculation.

The decay heat released by the fission products has an influence on the thermal hydraulic behaviour in the containment. Apart from its influence on fog formation and relative humidity, the decay heat also influences the atmosphere flows in the containment. With consideration of the decay heat, some COCOSYS calculations will come up with a more strongly mixed containment atmosphere than would be the case if the decay heat was not taken into account. The decay heat model uses the following assumptions: the decay heat released by beta and gamma radiation is considered; the beta radiation heats up the atmosphere, the sump and the outside layers of the considered structures; the fission products are assumed to be homogeneously distributed on the considered hosts; the radiation in the sump is fully absorbed [5].

2.13.3 Interlinkage to other codes in radiological consequences evaluation method

2.13.3.1 ATHLET
The thermal hydraulic code ATHLET is not designed for evaluation of radiological consequences. However, a coupling to the code DYN3D is available [10] (for description of DYN3D, see Section 2.5).

2.13.3.2 ATHLET-CD
The ATHLET-CD code does not have any explicit or implicit interlinkage/interface with any radiological consequences evaluation codes. The released fission products are transported through the primary circuit and discharged through the leak to the containment, which is simulated by COCOSYS (see next subsection).

2.13.3.3 COCOSYS
The COCOSYS code does not have explicit or implicit interlinkage/interface with any radiological consequences evaluation codes [5].

The radiological consequences of an accident in a nuclear reactor depend on the quantity of the radioactive material that escapes to the environment. As the radioactivity is transported through the containment and other buildings, credit is given for several natural and engineered removal mechanisms. Within compartments, these removal mechanisms include sprays, natural deposition, leakage, natural and forced convection, filters, and suppression pools.

The above aspects of formation and transport of the radionuclides are available for COCOSYS code within the containment boundaries. The received inventory of fission products in the reactor core and possible release to the containment (confinement for NPP with VVER 440/230), based on the maximum full-power operation of the core and the maximum period of irradiation, may be the COCOSYS code calculation result. These calculation results

(quantity and spectrum of the radionuclides, their distribution and time dependent behaviour, radionuclides activity) can be used for subsequent evaluation of the radiological consequences regarding to the environment beyond the boundaries of containment: using analytical assessment methods, e.g. given in guide [31]; preparation of initial data for further calculation using codes of the evaluation radiological consequences, e.g. MACCS and COSYMA (probabilistic risk assessment) as well as RASCAL/InterRAS3 and HOTSPOT (emergence response) [32].

2.13.4 Further development needs

2.13.4.1 ATHLET

No improvement of ATHLET is planned during the project. Statistical calculation sequence between ATHLET and TRANSURANUS (alternatively RELAP5 – TRANSURANUS) will be further developed by UJV.

2.13.4.2 ATHLET-CD

In the current approach, the core is modelled in a rather rough way by a limited number of concentric rings (typically 4-6). For each ring, a thermal-hydraulic channel is modelled and the fuel/control rods are modelled by one representative rod per section. It is planned, that a new approach of the core modelling is applied, which is currently being developed by GRS [1, 33]. With the new approach, the core can be sub-divided into a larger number of sections (also azimuthal subdivision). Furthermore, the current input deck of the Generic Konvoi PWR model will be updated in such a way that flow distribution during blow-down and reflood phase of the LOCA transient is simulated more accurately (e.g. analysis of cross flow friction loss coefficients). A more accurate calculation of the boundary conditions of the fuel rods is expected as outcome of this work.

Other possible improvements of ATHLET-CD will be performed in collaboration with code developer GRS. One of the current code limitations is that only one set of fuel parameters can be defined in the input (e.g. gas gap pressure). The dependence of gas gap pressure and other rod conditions on burnup is missing, which has a significant influence on cladding failure behaviour.

Development of data transfer between ATHLET-CD and JRodos will be developed.

2.13.4.3 COCOSYS

There are the following preferences regarding further development of the COCOSYS code [34-37]:

- further development of coupled calculation scheme with DET3D code for the simulation of hydrogen detonation taking into account recommendations to the DET3D model features;
- further development of iodine chemistry and behaviour model for the resuspension process on the mixing phase; expansion of the list of simulated iodine chemical reactions;
- improving the accuracy of modelling the following processes: Iodine adsorption and desorption on/from steel surfaces or walls painted with organic compounds; simulation accounting of the reaction of iodine and ozone; aerosol resuspension of depleted aerosols, e.g. in case of hydrogen combustion; molten corium-concrete interaction itself and the coupling to thermal hydraulics; modelling refinement of the direct containment heating;
- increase of the reliability of source term analyses;
- improvement of understanding, as well as an increase in the reliability of the simulation of the ex-vessel melt characteristic behaviour;
- BWR-specific modification and/or extension of the modelling;
- improvement in flexibility and expansion of the range of applicability of the interface between thermal hydraulic models (control volumes parameters feedback) of the COCOSYS calculation model and CFD (CFX) model; it should also be noted that recommendations regarding CFD model features are needed for coupled COCOSYS/CFX problems (spatial partitioning features, grid sampling rate, possible simplifications and assumptions for CFD model).

Developments for the COCOSYS code are not foreseen within the R2CA project.

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2.14 APROS

2.14.1 General overview of the code and modelling capabilities

The development of Advanced PROcess Simulation (APROS) software began in 1986 in co-operation between VTT Technical Research Centre of Finland Ltd. and Fortum Nuclear Services Ltd. The toolkit covers a wide range of functions from nuclear power plant simulator applications through chemical, thermal and nuclear engineering projects. The available model components enable the user to analyse the behaviour of systems with complex automation and thermal-hydraulic (TH) design. The TH model library contains three different TH models for one dimensional water/steam/gas flow (homogeneous, 5- and 6-equation), one for single phase flow, one for the containment and one for the steady state flow with tank dynamics. The TH is described using the conservation equations for mass, momentum and energy and correlations for friction and heat transfer. The performance of the Apros code has been validated extensively (more than 70 cases) by modelling various test facilities and comparing calculation results to a large set of measurements from selected transients. The TH models have been validated against a set of separate effect tests and integral tests (integral tests mean e.g. test facility experiments, such as ISPs - International Standard Problems). The TH and reactor models together with the automation system have been thoroughly tested by comparing calculation results with real plant data [1]. An advanced 3D multi-group neutronics model was implemented, based on HEXTRAN and HEXBU-3D nodal codes. Such approach using diffusion-theory mitigated the issues of the default finite-difference-based neutronics model in transients e.g. control rod ejection or boron dilution [2].

The nuclear library of Apros has a severe accident (SA) package that consists of four cooperating modules:

- GENFLO: the TH model of the reactor pressure vessel (RPV) [3]
- SARELO: the relocation model simulating the melting of the reactor core [4]

- COPOMO: the corium pool model simulating the behaviour of the melted reactor core inside the reactor pressure vessel [5]
- FIPROMO: the fission product model simulating the release and transfer of fission products and heat released from the fission products [6]

The subroutines of the SA package are not linked to the executable program of Apros, instead the subroutines are compiled and connected to an external library handled by the external model package of Apros. Depending on user preferences the GENFLO model can be replaced with the six-equation model of Apros in order to simulate the TH of the RPV. In this case the TH solution of all components is provided by Apros utilizing the enabled SA models (SARELO, COPOMO, FIPROMO).

The dose rate calculation of the SA package is executed in two steps: (1) activity calculation of 20 important isotopes (Kr, Xe, I, Cs and Te) and (2) dose rate conversion. Step (1) requires user input at the time of the reactor scram and the corresponding decay constants of the relevant isotopes. Step (2) offers two alternatives, namely the Radiation Calculation (RC) module requires user input for dose rate coefficients for each nuclide in each control volume in order to convert nuclide activities into dose rates. The other option is the Gamma Calculation module for simpler cases requiring node dimensions and shape factors, based on which the code calculates node-specific dose rates caused by a given source (volumetric or surface). The Apros SA dose rate model showed acceptable results compared to the SaTu model (Säteilyasiantuntijan Tukijärjestelmä, developed by Fortum [7]) considering an MBLOCA in the emergency core cooling system (ECCS) of a VVER-440 unit [8].

An extensive validation work has been carried out with the Apros CONtainment library (ACON) recently [9] considering hydrogen burning complementing the traditional TH features of the containment model. The burning model calculates continuous and discrete combustion of H_2 and CO_2 in the containment control volumes. Hydrogen igniters can be simulated via properties of the discrete combustion model e.g. setting time constraints and flammability limits. Passive autocatalytic recombiner (PAR) models are also available in the ACON library, the basic option utilizes a simplified form of the Arrhenius equation in order to calculate recombination rate [10]. The other option is based on a specific correlation of recombination capacity for Areva type PARs [11]. Nevertheless, both models can be adjusted according to user preferences by modifying a wide range of input variables.

2.14.2 Fission product (FP) release and FP transport modelling in the code

The node, branch and heat transfer variables needed for FP transport simulation are provided and updated by the corresponding Apros and/or GENFLO variables since the nodalization of the FP model is based on the TH and containment nodalization of the Apros base model. Required variables may be e.g. inlet and outlet liquid/gas mass flows, pressures, enthalpies, void fractions and hydrogen mass fractions. The heat flows from FPs to fluid and heat structures calculated by FIPROMO are passed onto the TH routines of Apros during the simulation while heat flows from the outer surface of the RPV to the containment nodes (calculated by the COPOMO module) are also updated in the TH solution representing feedbacks between SA and TH algorithms.

The FP transport calculation requires user-given properties in order to initialize the FIPROMO model. One of the first steps is setting the decay power (DP) curve for FPs, in case of SA calculations this function differs from the general one used in Apros TH calculations. The DP function has to be defined in time domain (W - s) as a discreet function, the program performs logarithmic fit between the points. Hereafter the DP densities (W/kg) have to be applied to each FP group, maximum 10 groups can be defined, by default the following 6 groups are used:

1. Noble gases (^{85m}Kr, ^{85}Kr, ^{87}Kr, ^{88}Kr, ^{133m}Xe, ^{133}Xe, ^{135m}Xe, ^{135}Xe, ^{138}Xe)
2. Iodine (^{131}I, ^{132}I, ^{133}I, ^{134}I, ^{135}I) and bromine
3. Caesium (^{134}Cs, ^{136}Cs, ^{137}Cs, ^{138}Cs) and rubidium
4. Tellurium (^{132}Te, ^{134}Te)
5. Other metallic FPs (e.g. Mo, Tc, Ru, Rh, Sb)
6. Other oxidic (non-metallic) elements (e.g. Ba)

The FPs are introduced to a node, branch or process component via the Fission Product Feed (FPF) module feeding mass fractions or mass flows of FPs. In both cases a two-dimensional array describes the properties where the first index refers to the location of the FP (in gaseous form, aerosols with various diameters, in spray droplets, deposited / in aqueous solution) and the second index refers to the number of the FP group. Aerosols may have 8 classes for different sizes, each with its own deposition velocity. The initialization of the SA calculation triggers a subroutine creating Fission Product Mass (FPM) modules for the process components included in the simulation, these modules store and process inlet/outlet FP mass information of the given node. The Fission Product Branch (FPB) module is used to solve FP mass flows between the FPM modules, these branches are also automatically created upon SA calculation initialization.

The SARELO module calculates the FP release from fuel by the following methodology: if the maximum cladding temperature of a core subchannel exceeds the temperature limit (set by the user) the cladding is considered to have ruptured. Hereafter a time-dependent Arrhenius equation determines the FP release rate. The FPs from the gas volume of the fuel rod are transferred to the adjacent TH nodes immediately after the rupture. The released isotopes are divided to gaseous group and aerosol particle groups according to a pre-determined distribution.

The retention of FPs is simulated on heat structures and water pools where aerosol removal rate is calculated from four deposition processes: gravitational deposition (sedimentation), turbulent impaction, thermophoresis and diffusiophoresis whereas Brownian diffusion is omitted. The effect of internal spray is also considered between spray droplets and aerosols via impaction, interception, thermophoresis and diffusiophoresis [12]. Note that no designated pool-scrubbing model is used at the moment, aerosol migration during solvent phase-change is solved with the corresponding TH transport models (condensation, boiling).

2.14.3 Interlinkage to other codes in radiological consequences evaluation method

Apros has been used in a previous analysis [13] [14] to provide TH and decay heat boundary conditions for the coupled fuel performance code FRAPTRAN-GENFLO, cf. Sections 2.9 and 2.2, and will be used for that purpose in R2CA project.

VTT has been developing the FINIX fuel behaviour module since 2012 [15], the code provides feedback on the fuel rod behaviour during transient conditions and extended irradiation periods. FINIX has been coupled to Monte Carlo and nodal diffusion solvers e.g. HEXTRAN [16]. Direct coupling of Apros-FINIX has not been realized so far due to a lack of necessity albeit soon to be launched development projects might consider this as an ultimate goal.

Another future application for Apros SA could be a coupling with the VALMA code (viranomaisten VALMiustoimintaan ja harjoituksiin sovitettu integroitu Annoslaskentajärjestelmä) that is a winding trajectory based off-site dose assessment tool using live weather data provided by the SILAM server of the Finnish Meteorological Institute [17].

2.14.4 Further development needs

Considering zirconium oxidation the Apros SA offers four correlations for reaction-rate coefficient calculation however these functions do not consider e.g. boron - stainless steel - zirconium interactions during core degradation which was highlighted as an important process by Di Giuli et al. [18]. Moreover, it was concluded that a better estimation of structural material release is needed, especially for tin from zircaloy cladding and for semi/low volatile FP release. An improved description of gaseous iodine behaviour in the RCS could also enhance computational capabilities taking into account the kinetics of iodine reactions in the primary system (e.g. Cs-I-B-O-H, Cs-I-Mo-B-O systems with B_4C). A collaboration between VTT and JAEA has started in 2017 addressing these issues by experiments at Finnish and Japanese facilities as support for JAEA's FP chemistry database development program [19], the results of the project are expected to be published soon.

Other relevant tasks could focus on developing in-vessel melt pool models (e.g. with Ag-In-Cd and oxidized SS), FP aerosol agglomeration into larger particles, corium - concrete interaction models and expanding chemistry

libraries. Shielding effect of water on containment floor has not been considered yet in the dose rate calculation leaving room for further improvement.

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2.15 ASTEC

2.15.1 General overview of the code and modelling capabilities

The ASTEC integral code (Accident Source Term Evaluation Code), has been jointly developed by IRSN (France) and GRS (Germany) from the late 1990s and is exclusively developed by IRSN today. ASTEC simulates an entire Severe Accident (SA) sequence in a nuclear water-cooled reactor from the initiating event through the release of radioactive elements out of the containment, including severe accident management by engineering systems and procedures [1-2]. ASTEC progressively became the reference European severe accident integral code for water-cooled reactors, in particular through the capitalization of new knowledge acquired in the frame of the SARNET European Network of Excellence from 2004 to 2013 (6th and 7th Framework Program of the European Commission) and in the CESAM project from 2013 to 2017 (7th Framework Program of the European Commission). Main ASTEC applications are therefore source term determination studies, level 2 Probabilistic Safety Assessment (PSA2) studies, accident management studies and physical analyses of experiments. It can be used for various types of 2nd and 3rd generation reactors (PWRs including VVERs, BWRs, and PHWRs including CANDU reactors).

The ASTEC code structure is modular, each of its modules simulating a reactor zone or a set of physical phenomena (see Fig. 2.11). A short description of the capability of each module is given hereafter.

2.15.1.1 CESAR module

The CESAR module simulates the thermal hydraulics (TH) in the primary circuit (including the reactor vessel) and in the secondary circuit. The TH modelling in CESAR is based on a 2D 2-fluid approach. Up to N non-condensable gases (hydrogen, helium, nitrogen, argon and oxygen) are available. In intact or slightly degraded meshes, a 5-equation approach is used; as a results, 5 + N differential equations and 1 algebraic equation (modelling the interfacial drag between the liquid and the gas phase) are solved. In degraded meshes and if parietal friction is large, a 6-equation model is used (two momentum equations, one for each fluid phase). Thermal and mechanical non-equilibrium are considered between phases. Specific swollen water level volumes are used to model large two-phase domains such as pressurizer. The following components can be represented: hydro-accumulators, pumps (which are described through a 0D approach), valves, breaks (with correlations for critical and sub-critical flow), pressurizer spray and heater systems. Most of the CESAR physical constitutive laws are issued from the correlations included in the French best estimate TH code CATHARE 2. In addition, a reflooding model is implemented which enables CESAR to simulate the reflooding of intact or degraded cores. The numerical method follows the finite volume technique. The space is discretized using a staggered grid with the use of the donor cell principle. The time integration is performed using a Newton's method and applying a fully implicit scheme. The Jacobian matrix inversion is based on a highly optimized Lower Upper algorithm, which makes CESAR a fast running and at the same time stable module.

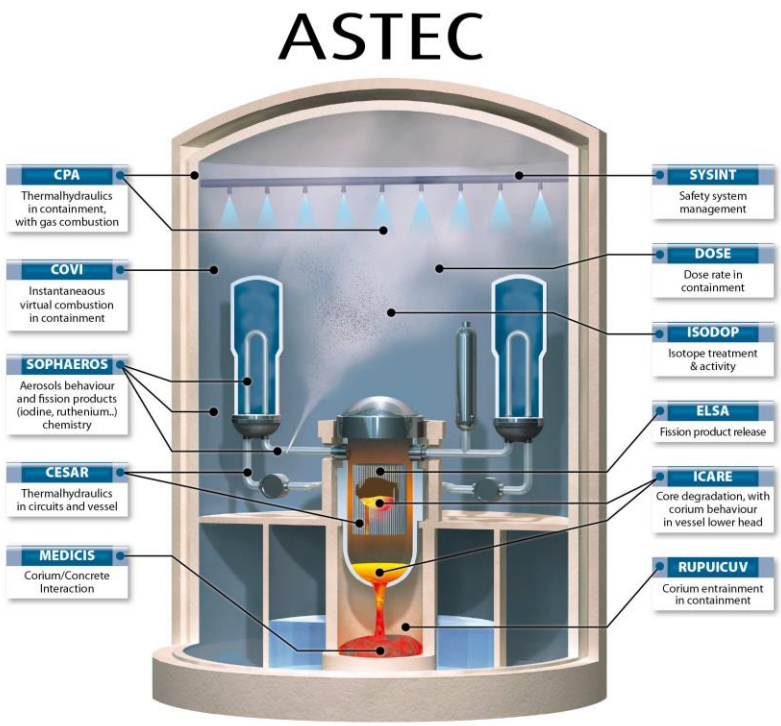

Figure 2.11. Modular code structure of ASTEC.

2.15.1.2 ICARE module

The ICARE module describes the in-vessel core degradation phenomena for both early phase (fuel rod heat-up, ballooning and burst, exothermic cladding oxidation, control rods behaviour, fuel rod embrittlement or melting, molten mixture candling and relocation…) and late phase (corium accumulation within the core channels and formation of blockages, corium slump into the lower head and corium behaviour in the lower head until vessel failure). The core is discretized in cylindrical rings (with the possibility of multi-channels meshing) and axial meshes in addition to a specific mesh for the lower head. Intact structures are described thanks to cylinders or square boxes components whereas degraded structures are modeled with debris (for broken or cracked structures) or magma (for molten materials) components. ICARE allows to compute heat transfers (by conduction, convection and radiation), power generated in a material, rod mechanics (ballooning, creep, burst and loss of integrity on using user-criteria), chemistry (steam and air oxidation of Zr, steam oxidation of stainless steel, B_4C and U-O-Zr magmas, dissolution phenomena), material melting and relocation, solid debris formation and collapse, formation and expansion of a molten pool. Moreover, a special coupling, based on a prediction–correction method, is applied between the CESAR and ICARE modules.

2.15.1.3 CPA module

The CPA module simulates the TH in the containment. The discretisation through a “lumped-parameter” approach (0D zones connected by junctions and surrounded by walls) simulates simple or multi-compartment containments (tunnels, pit, dome) with possible leakages to the environment or to normal buildings. Using the sources of steam, hydrogen, FP gases and aerosols from RCS provided by other modules of ASTEC, CPA calculates gas distribution, temperature field, pressure build-up, and gas (hydrogen and carbon monoxide) combustion. The TH state of a zone can be described either by the equilibrium model assuming water and atmosphere homogeneously mixed for saturated and superheated (no water) conditions or by the non-equilibrium model where deposited and airborne water are separately balanced.

2.15.1.4 SYSINT module

The SYSINT module allows the user to easily simulate the management of engineered safety features, such as safety injection systems, pressurizer spray and heaters, management of steam generators, containment spray system in direct or recirculation mode, hydrogen recombiners, etc.

2.15.1.5 DOSE module

The DOSE module, which was specifically implemented in ASTEC V2 to answer IRSN PSA2 requirements, aims at evaluating the dose rate in bulk gas phase for each zone of the containment, as well as the inner wall dose rate. The dose rates include β and γ radiation contributions relative to each isotope. Anyway, it has however to be underlined that, up to now, this module was only validated by comparison with dedicated IRSN codes.

2.15.1.6 ISODOP module

The ISODOP module simulates decay of FP and actinide isotopes in different zones of the reactor and of the containment. It starts the calculation using an initial isotope inventory generated by a dedicated code and allows estimating decay heat and activity in the core, in the RCS, in the containment and in the environment. The JEFF (Joint Evaluated Fission and Fusion) database dealing with ~3800 isotopes is available in the V2.1 version of ASTEC.

2.15.1.7 MDB library

The library Material Data Bank (MDB), shared by all ASTEC modules, groups together all material properties under a unique simple readable format. This includes: all simple materials of a water-cooled reactor (solid, liquid and gas) and associated usual properties (enthalpy, conductivity, density…); ideal chemistry (equilibrium reactions); iodine chemistry in containment (kinetics); FP isotopes (decay heat, transmutation rates…); complex materials such as molten corium. The MDB library includes all the recent research on the nuclear material properties done in international projects: for FP, CIT and ENTHALPY FP4 projects, and for corium OECD, RASPLAV and MASCA projects. The evaluation of corium properties is based on the NUCLEA database for corium thermo-chemistry. It also benefits from a continuous validation at IRSN of the database contents.

2.15.2 Fission product (FP) release and FP transport modelling in the code

2.15.2.1 ELSA module

The ELSA module, tightly coupled to the ICARE module, simulates the release of fission products and structure materials from the degrading core [3]. The ELSA modelling allows describing the release from fuel rods and control rods (that can be followed by the release from debris or magma components). The modelling is based on a semi-empirical approach and the physical phenomena taken into account are the main limiting phenomena that govern the release. For intact fuel rods and debris beds, the FP release is described according to the degree of fission product volatility, split in 3 categories: for volatile species (such as Xe, I, Cs, or Te), release is described by species intra-granular diffusion through UO_2 fuel grains; for semi-volatiles species (such as Ba or Mo), release is described by evaporation into inter-granular porosities and mass transfer processes; for low volatiles species (such as U or Pd), release is described by fuel volatilization treated as the vaporization of UO_3.

2.15.2.2 SOPHAEROS module

The SOPHAEROS module simulates fission products and structure materials transport and chemistry in the whole reactor, i.e. both in the RCS and in the containment [3]. An important modelling issue is the iodine transport and chemistry due to the deep radiological impact of this element. To simulate the transport of FP vapours and aerosols, the RCS and the containment are discretised in a 1D series of control volumes with the use of twelve different states: suspended vapours, suspended aerosols, condensed vapour on walls, deposited aerosols on walls, sorbed vapours on walls, liquid phase, painted dry walls, steel dry walls, concrete dry walls, painted wet walls, steel wet walls, concrete wet walls. One must note that the 6 latest states are specifically involving iodine chemistry in containment. In the RCS, the model for kinetics of gaseous phase chemistry addresses the Cs-I-O-H-Mo-B system [4-5]. The transport key-phenomena taken into account for the vapour-phase are FP and SM homogeneous and heterogeneous nucleation to form aerosol, vapour condensation/evaporation onto aerosols and walls and chemisorption of vapours on walls; for the aerosols, agglomeration, deposition mechanisms as well as pool scrubbing (to deal with the retention of aerosols in the secondary side of flooded steam generators in case of SGTR scenario) are modeled. In the containment, beside the transport of FP vapours and aerosols, several models are specifically addressing iodine and ruthenium behaviour [6-8]. As concerns iodine, around 40 phenomenological models are considered that focus on the predominant chemical reactions in sump, gas phase and at the interface

with surfaces. More precisely, it describes in a kinetic way (i.e. non-equilibrium) the chemical transformations of iodine in the reactor containment building, taking into account three kinds of reaction: thermal reactions, radiolytic reactions and mass transfer processes. As concerns ruthenium, the three predominant chemical reactions in gas phase are considered. Besides, to feed the SOPHAEROS module with adequate boundary conditions for the iodine chemistry in the sumps, a special module is now responsible in ASTEC V2.1 for pH evaluation in the sumps of containment.

2.15.2.3 SAFARI module

The SAFARI module is dedicated to the rapid simulation of activity transfer from primary circuit to secondary and environment in a SGTR accident. It has a simpler approach than SOPHAEROS: The RCS nodalization is limited to a few zones (one for primary, one for each steam generator…), in which mass conservation equations of fission products are solved, taking into account transport by carrier fluid as well as other phenomena (deposition/resuspension, filtering, partition between phases) via coefficients. From the calculated mass transfers of FP, the isotope transport and transmutation is calculated, along with the activity.

2.15.3 Interlinkage to other codes in radiological consequences evaluation method

The ASTEC modules communicate with each other through a "dynamic" memory and data are exchanged between the ASTEC modules at macro-time steps through this dynamic database. Any module can be deactivated, provided that the variables which would be supplied to the database by that module, and which are required as boundary conditions for other modules, are given as an input of the calculation (in the form of time tables). For example, if a highly detailed calculation of core degradation including FP release is available, it can be chained to an ASTEC calculation where ICARE (core degradation) and ELSA (FP/SM release from the core) modules are deactivated: SOPHAEROS (FP/SM transport in RCS and containment) will then need the time evolution of FP released from the core to the primary to be provided as input.

2.15.4 Further development needs

The semi-empirical approach adopted in ELSA module (FP/SM release from the core) has been designed for severe accident conditions, characterized by high temperatures. It might need a reassessment for the more limited conditions of DBA.

Similarly, the models for iodine chemistry in containment developed in the context of severe accident conditions. In this case the effective conditions encountered in LOCA, in particular dose rate, have to be evaluated.

Regarding SGTR, the SOPHAEROS models concerning the iodine chemistry in the primary circuit, and the partition of iodine following the jet flashing at SGT breach have to be improved.

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2.16 MELCOR

2.16.1 General overview of the code and modelling capabilities

MELCOR is a fully integrated, engineering-level computer code whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. Current uses of MELCOR include estimation of fission product source terms and their sensitivities and uncertainties in a variety of applications see Refs. [1] to [5].

The MELCOR code is composed of an executive driver and a number of major modules, or packages, that together model the major systems of a reactor plant and their generally coupled interactions. Reactor plant systems and their response to off-normal or accident conditions, see Figure 2.12.

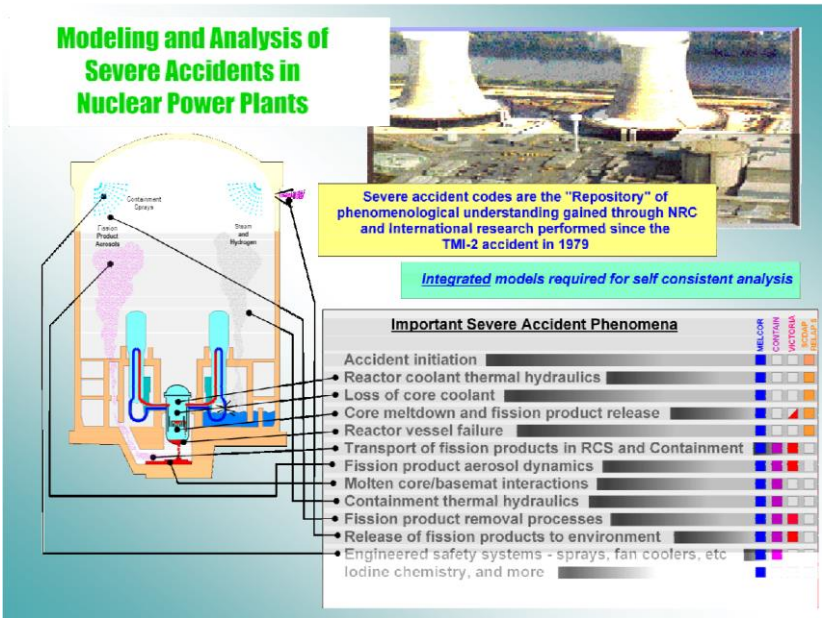

Figure 2.12. MELCOR severe accident phenomena.

Current uses of MELCOR often include uncertainty analyses and sensitivity studies. To facilitate these uses, many of the mechanistic models have been coded with optional adjustable parameters. This does not affect the mechanistic nature of the modelling, but it does allow the analyst to easily address questions of how particular modelling parameters affect the course of a calculated transient. Parameters of this type, as well as such numerical parameters as convergence criteria and iteration limits, are coded in MELCOR as sensitivity coefficients, which may be modified through optional code input.

2.16.2 Fission product (FP) release and FP transport modelling in the code

The RadioNuclide (RN) package models the behaviour of fission product aerosols and vapours and other trace species, including release from fuel and debris, aerosol dynamics with vapour condensation and revaporization, deposition on structure surfaces, transport through flow paths, and removal by engineered safety features. The package also allows for simplified chemistry controlled by the user.

MELCOR addresses those fission products (and daughters) released during an accident, which are particularly important for determining consequences and risks. MELCOR treats the molecular forms of all important fission products and also models the transport of all nonradioactive masses (water and concrete or other structural aerosols) with which fission products may interact.

Rather than tracking all fission product isotopes, the masses of all the isotopes of an element are modelled as a sum; that is, the total element mass, not its individual isotopes, is modelled. Furthermore, elements are combined into material classes, groups of elements with similar chemical behaviour, see Table 2.4.

Release of radionuclides can occur from the fuel-cladding gap by exceeding a failure temperature criterion or losing intact geometry, from material in the core using the various CORSOR empirical release correlations based on fuel temperatures, and during core-concrete interactions in the reactor cavity using the VANESA release model.

The aerosol dynamics models are based on MAEROS, a multisection, multicomponent aerosol dynamics code, but without calculation of condensation. Aerosols can deposit directly on surfaces such as heat structures and water pools, or can agglomerate and eventually fall out once they exceed the largest size specified by the user for the aerosol size distribution. Aerosols deposited on surfaces can be vaporized (if they are volatile) but can only be resuspended if the resuspension model is enabled.

The condensation and evaporation of radionuclide vapours at the aerosol surfaces, pool surfaces, and heat structure surfaces are evaluated by the rate equations from the TRAP-MELT2 code.

The amount of steam condensed or aerosol water evaporated is calculated by thermodynamics routines called by the Control Volume Hydrodynamics (CVH) package.

Models are available for the removal of radionuclides by pool scrubbing, filter trapping, and containment spray scrubbing. The pool scrubbing model is based on the SPARC code, and treats both spherical and elliptical bubbles. The model includes condensation at the pool entrance, Brownian diffusion, gravitational settling, inertial impaction, and evaporative forces for the rising bubble.

Chemistry effects can be simulated in MELCOR through the class reaction and class transfer models, which are controlled entirely by user-specified parameters.

Table 2.4. Default Radionuclide Classes and Member Elements[1]

Class Number and Name	Member Elements
1. Noble gases	Xe, Kr, (Rn), (He), (Ne), (Ar), (H), (N)
2. Alkali Metals	Cs, Rb, (Li), (Na), (K), (Fr), (Cu)
3. Alkaline Earths	Ba, Sr, (Be), (Mg), (Ca), (Ra), (Es), (Fm)
4. Halogens	I, Br, (F), (Cl), (At)
5. Chalcogens	Te, Se, (S), (O), (Po)
6. Platinoids	Ru, Pd, Rh, (Ni), (Re), (Os), (Ir), (Pt), (Au)
7. Transition Metals	Mo, Tc, Nb, (Fe), (Cr), (Mn), (V), (Co), (Ta), (W)
8. Tetravalents	Ce, Zr, (Th), Np, (Ti), (Hf), (Pa), (Pu), (C)
9. Trivalents	La, Pm, (Sm), Y, Pr, Nd, (Al), (Sc), (Ac), (Eu), (Gd), (Tb), (Dy), (Ho), (Er), (Tm), (Yb), (Lu), (Am), (Cm), (Bk), (Cf)
10. Uranium	U
11. More Volatile Main Group Metals	(Cd), (Hg), (Pb), (Zn), As, Sb, (Tl), (Bi)
12. Less Volatile Main Group Metals	Sn, Ag, (In), (Ga), (Ge)
13. Boron	(B), (Si), (P)
14. Water	(Wt)
15. Concrete	(Cc)
16. Cesium Iodide	(classes 2 and 4)

2.16.3 Interlinkage to other codes in radiological consequences evaluation method

MELCOR can be externally coupled with MACCS [6], a consequence analysis code, with a standard process which was developed to digest each of the MELCOR source terms in a consistent fashion, see Figure 2.13. MACCS can be used also as standalone, provided that the source term input is available.

MELCOR source terms output file in form of classes can be transformed as radionuclide input of MACCS by means of MELMACCS. In particular, MELMACCS extracts information from the MELCOR plot file and converts it into MACCS input values. To correctly interpret the MELCOR results, MELCOR mass values has to be associated with an ORIGEN output that allows masses of chemical classes to be converted to activities of individual radionuclides. Furthermore, the user has to select the chemical classes that are to be included in the analysis, provide an estimation of aerosol deposition velocities, and the timeframes to be used for each plume segment.

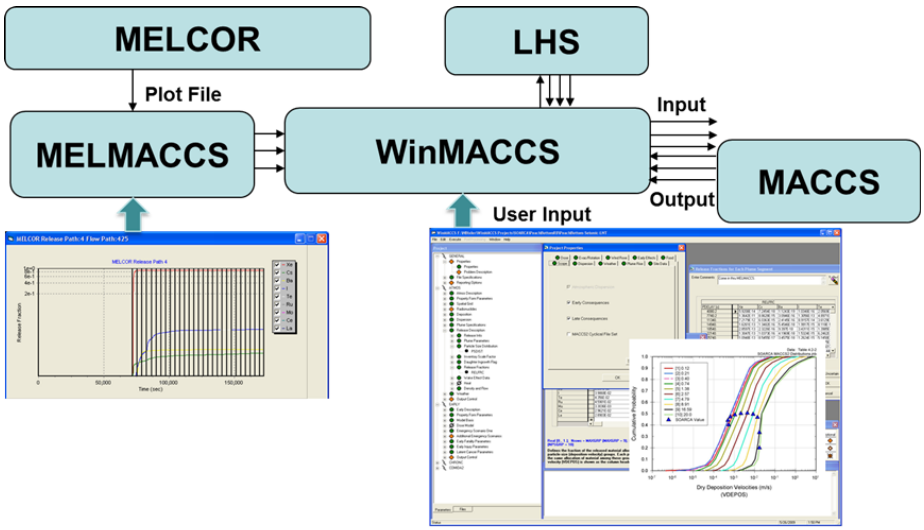

Figure 2.13. MELCOR and MACCS coupling.

[1]Enclosed in parentheses are the elements that do not contribute significant decay heat (< 1%).

2.16.4 Further development needs

The following further development needs are identified by the MELCOR Peer Review in [1]:

- RCS Deposition: omission in some aerosol deposition processes, principally inertial impaction and turbulent deposition. These processes, which are not generally important in containment, may assume primary importance in the reactor coolant system.
- Chemical Reactions with Surfaces: lack of explicit modelling for chemical reactions between deposited fission products and structures in the primary system. Such reactions can greatly affect deposition (chemisorption) and revaporization rates.
- Aqueous Chemistry: fission product chemistry in water pools is a less critical but still important modelling omission. The chief concern is that release of iodine to the environment may be understated because MELCOR neglects processes that can occur in water pools to transform cesium iodide into more volatile forms of iodine (e.g., reaction with methane to form methyl iodide).

Within R2CA, MELCOR code development is not foreseen, but new development needs may emerge as a result of the project.

2.16.5 References

[1] MELCOR Computer Code Manuals Vol. 1: Primer and Users' Guide Version 2.2.14959, SAND2019-12536 O, October 2019
[2] MELCOR Computer Code Manuals Vol. 2: Reference Manual Version 2.2.14959, SAND2019-12537 O, October 2019
[3] MELCOR Computer Code Manuals Vol. 3: MELCOR Assessment Problems Version 2.1.7347 2015, SAND2015-6693 R, August 2015
[4] MELCOR Code Change History: Revision 11932 to 14959, SAND2019-12533, October 2019
[5] MELCOR Best Practices as Applied in the State-of-the-Art Reactor Consequence Analyses (SOARCA) Project, NUREG/CR-7008, August 2014
[6] MACCS Best Practices as Applied in the State-of-the-Art Reactor Consequence Analyses (SOARCA) Project, NUREG/CR-7009, August 2014

2.17 JRodos

2.17.1 General overview of the code and modelling capabilities

JRodos is a Java based code, which is a follow up of RODOS, a real-time online decision support system for nuclear emergency management and rehabilitation issues after nuclear accident, which has been developed by the European Commission for more than three decades. The code itself is a property of The RODOS Consortium, which is represented by the KIT.

The models, together with a worldwide database and the supported coupling to a set of globally applicable meteorological weather forecast data allows real time general application for any point on the globe. The codes inherent features and tools allow the adaptation of models, databases as well as the user interface to national conditions and user preferences.

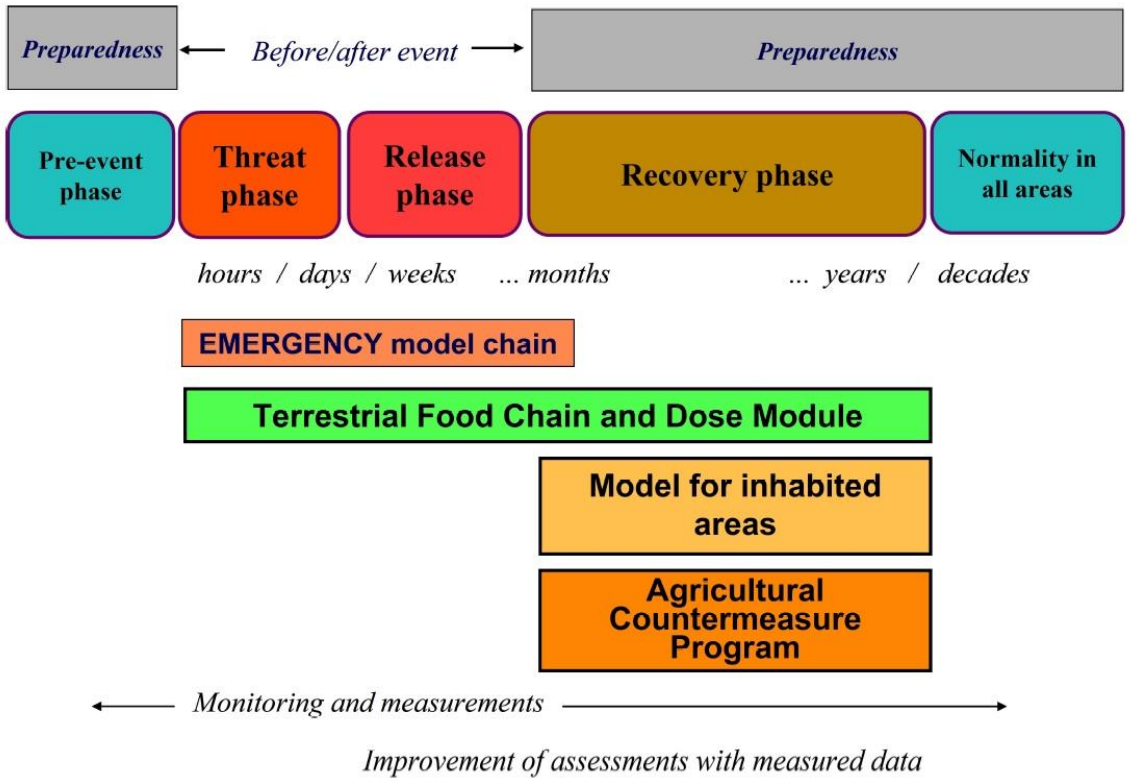

Figure 2.14. The JRodos models and model chains and the covered phases [1].

The JRodos simulation models cover typical terrestrial and aquatic exposure situations as well as several special situations. An overview of the models and model chains including phases they cover is presented in Figure 2.14. The atmospheric models can be distinguished in two main parts, the early and later phase models, where the countermeasures for interrupting or mitigating the early phase exposure pathways are sheltering, evacuation and the intake of iodine tablets. The transfer of radioactive fission products to food and subsequently to man is modelled by Terrestrial Food Chain and Dose Module, where, for the early phase, the module uses the radionuclide concentrations in the air near ground as an input, as well as information about the rainfall from the near or far range Atmospheric Dispersion and Deposition models. The phenomena considered in the food chain assume the airborne activity deposition onto the ground and vegetation by wet and dry deposition processes. The deposition process as well as the processes following afterwards depend on the seasonal development significantly. An uptake of activity by life stock via feed, watering and inhalation is considered as well as a follow-up biological transport and excretion processes, which lead to contamination of animal food stuffs. The original activity of raw products is changed before the consumption by various processing like simple washing or peeling as well as the conversion to secondary product, such as grain to flour.

The later phase models deal with the deposition onto natural and man-made surfaces and food contamination, which persists for months, years or even decades. The JRodos Model for Inhabited Areas takes processes of urban surfaces and surroundings contamination, and the related countermeasures like long-term evacuation, decontamination or a complete removal of the contaminated surface into account. Based on the initial deposition as an input, the model calculates the distribution in time over the different components of the urban environment. The corresponding Agricultural Countermeasure Program considers the contamination of agricultural areas and food and feed stuff together with a range of possible countermeasures from restrictions in food marketing over removal or decontamination actions to changing agricultural practices.

The Hydrological Model Chain models the aquatic transport and aquatic exposure pathways, which consists of dispersion of the released activity into and through most of the aquatic environments such as rivers, reservoirs, lakes or the open sea. The Aquatic Food Chain and Dose Models simulate the radionuclides transfer from contaminated water and fish to man and the resulting radiation exposure. The usage of contaminated water for

drinking and watering life stock and irrigating crops is considered. The user can, according to the modelled situation, choose from various models, e.g. a 3D model for deep reservoirs or a 1D for a river flow. All the aquatic models describe special situations and require more customisation to the target regions of application.

2.17.2 Fission product (FP) release and FP transport modelling in the code

The application of the JRodos code within the R2CA project is aimed at the calculation of the dose rate. The area of interest of the fission product transport is mainly in the atmosphere, where specific conditions for a specific nuclear power plant and country shall be applied.

The chain of basic models (LSMC+EMERSIM+DEPOM+FDMT) is used for calculation of FP transport through the atmosphere and biosphere (food chain), and the dose for representative person. The LSMC (Local Scale Model Chain) consist of ADM (Atmospheric Dispersion Model) and source term and meteorological data pre-processors used for calculation of the near range atmospheric dispersion of released FP. The DEPOM model is used for calculation of dry and wet deposition of FP on various surfaces. The FDMT calculates the dose for representative person from terrestrial exposure pathways (e.g. external irradiation from surface and plume, internal exposure from inhalation, ingestion and resuspension).

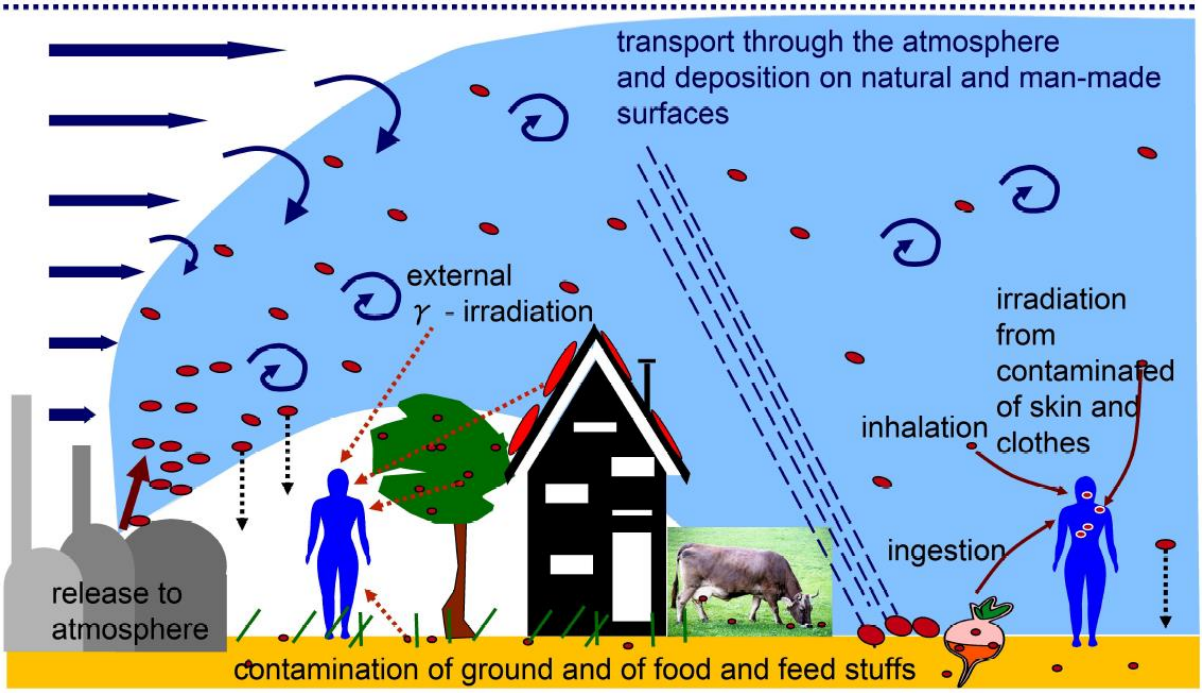

Figure 2.15. Atmospheric transport and deposition phenomena and terrestrial exposure pathways [1].

2.17.3 Interlinkage to other codes in radiological consequences evaluation method

The JRodos is a standalone code, no coupling is necessary due to the aim of the code.

The input of the JRodos code consists of several files, depending on the application purpose, e.g. the source term, initial inventory etc. The source term format is accepted in various forms, e.g. isotopic release in becquerel, mass fraction release for various radio isotopic groups. Furthermore, JRODOS can handle the IRIX format, i.e. import and export of the source term is available.

The initial and boundary conditions are the source terms, including the height of the release and buoyancy. The time domain is in the scale of hours, thus more precise definition of the source term is unnecessary.

2.17.4 Further development needs

It is not expected to develop the code within the framework of the R2CA project. The development will be in the data exchange with other codes, namely the AC^2 package. More specifically, a special software tool for data transfer between ATHLET-CD (part of AC^2) and JRodos will be developed. Some further development needs may arise from the JRodos code application.

2.17.5 References

[1] Karlsruhe Institut of Technology (KIT): JRodos: An off-site emergency management system for nuclear accidents;2017; Karlsruhe Institut of Technology (KIT)

[2] Søren Thykier-Nielsen, Sandor Deme, Torben Mikkelsen: Description of the Atmospheric Dispersion Module RIMPUFF; 1999; Risø National Laboratory

2.18 FEMAXI-6

2.18.1 General overview of the code and modelling capabilities

FEMAXI-6 code [1] can analyse the integral behaviour of the whole fuel rod throughout its life as well as the localized behaviour of a small part of a fuel rod. The code is designed mostly for the analysis of the normal operation. FEMAXI-6 consists of two main parts (see Fig. 2.16): one for analysing the temperature distribution, thermally induced deformation, and a fission gas release (FGR), etc., and the other for analysing the mechanical behaviour of the fuel rod. Temperature distribution, radial and axial deformations, FGR, and inner gas pressure are calculated as a function of irradiation time and axial position. Stresses and strains in the pellet and cladding are calculated and pellet-cladding mechanical interaction analysis is performed. Also, thermal conductivity degradation of pellet and cladding waterside oxidation are modelled. Its analytical capabilities also cover the boiling transient anticipated in boiling water reactor (BWR). Elasto-plasticity, creep, thermal expansion, pellet cracking and crack healing, relocation, densification, swelling, hot pressing, heat generation distribution, FGR, pellet-cladding mechanical interaction, cladding creep and oxidation are modelled by the code [1].

In FEMAXI-6 internal structure, finite element method based mechanical analysis and thermal analysis have a coupled solution using iteration in each time step for an accurate prediction of fuel behaviour, particularly in high burnup region. More precisely, the temperature and fission gas calculation use the gap size and contact pressure, which have been obtained by the mechanical analysis of entire fuel rod length. FEMAXI-6 code can perform a local pellet-cladding mechanical interaction analysis, such as pellet ridging as an optional process [1].

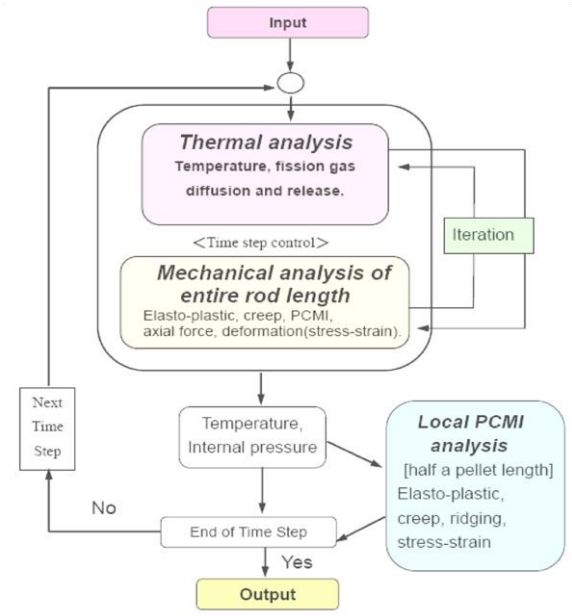

Figure 2.16. Entire code structure of FEMAXI-6.

Lithuanian Energy Institute (LEI) has used FEMAXI code for the modelling of the processes in the RBMK-1500 reactor for the LOCA accident [2]. The main conclusion of the work was that FEMAXI code cannot be applied for the analysis of LOCAs without special treatment of the steam starvation situation, which occurs during the LOCA. By calculating the heat transfer coefficients with RELAP5 and by taking FEMAXI's limitations into account, it is possible to evaluate the fuel rod behaviour in LOCA with the FEMAXI code. However, FEMAXI did not indicate the cladding rupture, and for that reason, a simple rupture criterion dependent on temperature and pressure difference was developed [2].

2.18.2 Fission product (FP) release and FP transport modelling in the code

FEMAXI has a model for FGR [1], but as it is a fuel performance code, FP transport outside the fuel rod domain is not considered.

2.18.3 Interlinkage to other codes in radiological consequences evaluation method

According to preliminary plan of LEI for R2CA, a calculation chain RELAP5 (alternatively: ASTEC) → FEMAXI (alternatively: TRANSURANUS) → ASTEC could be used. In the beginning, RELAP5 (or ASTEC) will be used for the TH calculations, and most importantly for the calculation of heat transfer coefficients to be used with FEMAXI. FEMAXI is used to evaluate the processes in the fuel and to evaluate the cladding integrity in similar fashion as done with the RBMK fuel in [2]. FEMAXI results will then be used with ASTEC, which will be used for the subsequent evaluation of releases from the RPV to the containment and from the containment to the environment. The above described calculation procedure has not been used before, and no coupling or interface for data transfer between FEMAXI and ASTEC currently exists.

2.18.4 Further development needs

Calculation procedure of using FEMAXI results with ASTEC has not been used before, and no coupling or interface for data transfer between FEMAXI and ASTEC currently exists. Data transfer capabilities in the calculation chain described in Section 2.18.3 should be implemented.

2.18.5 References

[1] Suzuki M., 2005. Light Water Reactor Fuel Analysis Code FEMAXI-6 (Ver. 1). Japan Atomic Energy Research Institute

[2] Jusevičiūtė A., Kaliatka A., Urbonavičius E., Duškesas G., Juodis L., Sonnenburg H.G., 2008. Assessment of FEMAXI and TESPA-ROD codes for modelling of BDBA in RBMK-1500. Kerntechnik, ISSN 0932-3902, Vol. 73, No. 4, pp. 197-206

2.19 FRAPCON

2.19.1 General overview of the code and modelling capabilities

FRAPCON is a single rod fuel performance code developed by Pacific Northwest National Laboratory (PNNL) for the U.S. Nuclear Regulatory Commission (NRC) and intended for steady-state and power ramp analyses [1]. FRAPCON has been written with the Fortran 90 standard, and it originates from the same code family as the transient fuel performance code FRAPTRAN [2]. In LOCA analyses, FRAPCON is used to initialize the transient calculations performed with FRAPTRAN. The latest FRAPCON version is 4.0 patch 1, released in 2015, and it is intended to be replaced by the U.S. NRC's FAST code [3] which is a merger of FRAPCON and FRAPTRAN.

FRAPCON-4.0 has been validated for PWR and BWR reactors up to rod average burnups of 62 MWd/kgU [4]. The maximum heat generation rates in the validation database are up to 60 kW/m, rearched in the beginning of the irradiation [4]. The modelled pellet materials include UO_2, MOX, UO_2 with gadolinia additive, and UO_2 with ZrB_2 coatings, and the cladding types include Zircaloy-2, Zircaloy-4, ZIRLO™, Optimized ZIRLO™ and M5™ [1]. The code can be used to evaluate fuel and cladding temperatures, rod internal pressure, FGR, cladding deformation, corrosion and hydriding. FRAPCON and FRAPTRAN have common fuel and cladding thermal and mechanical material properties [5] which are based on the MATPRO material properties package [6].

The code applies finite difference method for the heat conduction modelling and the mechanical model FRACAS-I which is also used in FRAPTRAN. There is also a finite element mechanical model available but it has not been validated by the code developers. The fuel rod is divided into axially stacked slices with radial noding, and any azimuthal variation is not considered. For the fuel, FRACAS-I is a so-called rigid pellet model, i.e., it does not consider stress-induced deformation of the fuel. FRACAS-I can handle only small cladding deformations, i.e., less than 5% [1]. The bulk coolant temperature is calculated with a single-channel coolant enthalpy rise model [1].

There is a built-in sensitivity analysis capability in FRAPCON. Eight model parameters have been chosen based on a sensitivity study [7]: fuel thermal conductivity, fuel thermal expansion and swelling, FGR, irradiation creep, cladding thermal expansion, corrosion and hydrogen pickup [1]. Bias can be set for each of those models via input but the standard deviations of the models have been hardcoded into the code.

FRAPCON has refabrication capability that enables continued simulation of a segmented rodlet in a research reactor. The option enables changing, e.g., the internal gas pressure and composition, and plenum dimensions.

2.19.2 Fission product (FP) release and FP transport modelling in the code

FRAPCON calculates the generated total fission gas at given axial elevation as a function of burnup and production rate of krypton, xenon and helium. Besides FGR, FRAPCON considers the release of nitrogen trapped in fuel during the manufacturing. There are four FGR options in FRAPCON, all based on the Booth formalism [8]: ANS-5.4 [9] and updated ANS-5.4 [10], Massih model [11] modified by PNNL, and the so-called FRAPFGR model developed by PNNL [1]. The default and recommended FGR model is the Massih model which is reported [1] to give best predictions on stable FGR compared to the other models. However, the Massih model cannot provide the information on distribution of fission gases in the pellets (radial, inter- and intragranular) prior to a RIA transient simulated with FRAPTRAN, and therefore the FRAPFGR model has been developed. The ANS-5.4 model is used in evaluation of the release of radionuclides with short half-lives [1]. As FRAPCON is a single rod fuel performance code, there is no FP transport model beyond the calculation domain of a fuel rod.

The pellet radial noding for the gas release calculation is different from that of the thermal calculation; the radial rings have equal volume in gas release calculations whereas in temperature calculations, the code divides the periphery of the pellet into higher number of nodes in order to obtain more realistic radial temperature profile.

2.19.3 Interlinkage to other codes in radiological consequences evaluation method

The coolant boundary conditions are specified by the inlet temperature, pressure, mass flow rate and channel geometry. The axial linear heat generation rate history is also needed, as well as the fuel manufacturing parameters. Various neutronics codes can be used to obtain the power history.

FRAPCON produces a restart file to be used with FRAPTRAN in transient and accident simulations. The restart file contains various base irradiation data items such as cladding plastic strain, burnup distribution, moles of gas in the rod and the composition of the gas, cladding outer surface oxide thickness, cladding hydrogen concentrations, fuel open porosity, fuel displacement due to swelling and densification, etc.

2.19.4 Further development needs

As FRAPCON is a steady-state code, no major FRAPCON code developments are foreseen in R2CA as the project is dedicated for modelling LOCAs and SGTRs. Regarding the cladding characterization before the transient, a model of hydrogen migration/precipitation of secondary hydrogen uptake under operations conditions of defective fuel rods will be coupled with FRAPCON, so that cladding embrittlement will be better estimated.

2.19.5 References

[1] Geelhood, K.J., Luscher, W.G., Raynaud, P.A., Porter, I., 2015. FRAPCON-4.0: A computer code for the calculation of steady-state, thermal-mechanical behavior of oxide fuel rods for high burnup. PNNL-19418, Vol.1 Rev.2

[2] Geelhood, K.J., Luscher, W.G., Cuta, J.M., Porter, I., 2016. FRAPTRAN-2.0: A computer code for the transient analysis of oxide fuel rods. PNNL-19400, Vol.1 Rev2

[3] OECD/NEA, 2019. Updated LOCA state-of-the-art report, November 2019 draft version

[4] Geelhood, K.J., Luscher, 2015. FRAPCON-4.0: Integral assessment. PNNL-19418, Vol.2 Rev.2

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[10] ANS, 2011. Method for Calculating the Fractional Release of Volatile Fission Products from Oxide Fuel. ANS5.4 of the Standards Committee of the American Nuclear Society (ANS), ANSI/ANS-5.4-2011

[11] Forsberg, K., Massih, A.R., 1985. Diffusion theory of fission gas migration in irradiated nuclear fuel UO_2. Journal of Nuclear Materials Vol. 135

2.20 FUROM

2.20.1 General overview of the code and modelling capabilities

The code FUROM has been developed for the computational simulation of VVER and PWR fuel behaviour in quasi-static conditions. Special attention was given to the validation of the code by using experimental results from international sources. The code is used for the systematic evaluation of the fuel-related safety parameters of Paks NPP on a regular basis.

The code is a finite difference code based on the quasi-static approach, i.e. no time dependence is taken into account within one time step. The scope of the code is therefore limited to normal operation processes and anticipated operational occurrences, where changes are not too abrupt for the quasi-static approach to be applicable. Within this scope time steps are automatically sub-divided to limit the time elapsed in one step or the power change between consecutive time steps.

The code performs 1.5D simulations, i.e. cylindrical geometry and azimuthal symmetry of boundary conditions, power distributions, material data, stresses and strains are assumed and the radial and axial characteristics of the fuel rod are calculated for discrete radial rings in discrete axial sections. The input required by the code consists of the fabrication parameters, the history and the selection among model parameter options.

The radial burn-up and power profiles, including profiles for different gadolinium contents, are approximated by burn-up dependent polynomials previously fitted to neutron physics calculations that take into account all significant neutron physics effects, e.g. self-shielding of resonance capture by ^{238}U.

The thermo-mechanical behaviour of the fuel is calculated in each time step starting from the coolant and progressing inwards, in two embedded iteration loops: one solving the complete thermo-mechanical problem for each axial section and one coupling the results of all the axial sections by the effect of fission gas release and the resulting rod pressure.

Heat transfer between the coolant and the cladding, across the cladding and across the gap is taken into account as a temperature jump each. Thus one obtains the pellet surface temperature. Then the heat conduction equation is solved ring by ring for the pellet, ignoring heat transfer between axial sections.

Pellet deformations are calculated neglecting elastic and plastic deformations and creep (this is referred to as rigid pellet model). Cladding deformations are considered using the incremental deformation model. Cladding deformation is caused by several phenomena: thermal expansion, irradiation growth, difference between the external and internal pressure (causing elastic and plastic deformation and creep). The calculation of a free-standing cladding basically differs from the calculation of the closed-gap situation. For a free-standing cladding, the above contributions are calculated and the result is determined by the creep-stress iteration. When the gap is already closed in one or more axial nodes then an extra axial stress is taken into account for the nodes with free-standing cladding below the closed-gap nodes. When the gap is closed and the axial force exerted by the contact pressure exceeds the above axial tensile force then it is assumed that the axial deformation of the cladding section is identical to the axial deformation of the fuel stack section (sticking occurs). When the gap is closed but the axial force exerted by the contact pressure is less than the axial tensile force then two model options are available: in the sliding model sliding occurs and the deformation of the cladding section is calculated from this condition, while in the sticking model the axial deformation of the cladding section is identical to the axial deformation of the fuel stack section.

The code has been validated against experimental results. Some results calculated by other codes were also used for benchmarking. The quantities used during validation were fuel centreline temperature, axial deformation of the fuel stack, axial deformation of the cladding, radial deformation of the cladding, thickness of the oxide layer, hydrogen absorption of the cladding, fission gas release, isotope concentrations in the free volume, internal pressure.

2.20.2 Fission product (FP) release and FP transport modelling in the code

Fission gas generation is a basic phenomenon that influences fuel behaviour during burn-up. The number density of each fissile species and fission product changes with burn-up, which has to be accounted for. This is more complicated in fuel rods containing gadolinium, as the strongly space-dependent change of gadolinium isotope concentrations significantly influences the phenomena. A certain portion of gaseous and volatile fission products does not remain in the fuel matrix but is released from the fuel grains. The release of fission products from the fuel material significantly increases at higher burn-up.

The production and release of the 33 most important fission products (including 8 stable nuclei) are calculated by the code. The number densities of actinides and fission products are calculated first for the axial nodes, then the actual number densities of fission products are determined for each radial ring in every axial node assuming that the production of short-lived isotopes is proportional to the local linear heat rate, while the production of long-lived isotopes is proportional to the local burn-up. Using the space-dependent distribution of isotope concentrations, the release of gaseous and volatile fission products into the free volume is calculated. Several release models are implemented in the code. Thermal release is calculated either by an effective one step model or, alternatively, by a two-step model. In the one-step model the fission products released from the grains appear instantaneously in the free volume without the formation of inter-granular bubbles, whereas in the two-step model they are released first from the grains to inter-granular bubbles and only after an incubation time into the free volume. The a-thermal release due to the high burn-up structure is modelled by two alternative models. However, only the krypton and xenon noble gases contribute to the internal pressure, as volatile isotopes condense or undergo chemical reactions in the gap.

2.20.3 Interlinkage to other codes in radiological consequences evaluation method

The code writes two output files to be further used by the code TSKGO. One of them consists of the rod average burnup, rod internal pressure, the gap inventory of helium and of the stable isotopes of krypton and xenon (in atoms) and the gap activity of the 25 radioactive krypton, xenon, bromine, rubidium, iodine and caesium isotopes in each time step. The other one consists of rod average/total quantities and quantities given for each axial section in each time step. The rod average/total quantities are burnup, LHR, internal pressure, total free volume, average gas temperature, helium, krypton and xenon content (in atoms) and the total release rate of the above mentioned 33 nuclei. The axially listed quantities are burnup, LHR, gap volume, central hole volume and the local release rate of the 33 nuclei. These data are used by the code TSKGO as described in the corresponding section.

The code also writes an output identical to a FRAPCON output, to be used by the FRAPTRAN code.

The code does not use the results of more detailed codes in the form of any coupling.

The code needs the cooling temperature and pressure history during normal operation as its boundary conditions. The temperature history is ideally the local cladding temperature in all axial sections or the coolant temperature in all axial sections, or if neither of these is available, then the inlet and the outlet temperature of the fuel rod, or ultimately for VVER-440 reactors only the core inlet temperature.

2.20.4 Further development needs

No code development is foreseen for the code FUROM in the framework of the R2CA project, as it only provides input data for the codes that simulate transient fuel behaviour.

2.20.5 References

[1] János Gadó, Ágnes Griger, Katalin Kulacsy: The fuel behaviour code FUROM and its high burn-up simulation capabilities, Nuclear Engineering and Design 327 (2018) 274–285

3. Model comparison charts

In order to compare various models of the codes used in the R2CA project, questionnaire chart templates were formulated. Special attention was given to modelling of fission product behaviour. As there are codes with different modelling scales, the template was divided into two tables: fuel performance / radionuclides behaviour codes in one table, and integral system codes / thermal hydraulics codes in the other.

Concerning JRodos, the template was left unfilled as no other similar codes modelling the radiological consequences outside the containment are used in the project. As EdF and LEI are not taking part to Task 2.1.2, MAAP and FEMAXI-6 were not considered.

The filling instructions of the tables were:

- Most of the questionnaire consists of checkboxes, in which it should be filled if the specific phenomenon is modelled or not in the code
- Mark 'X' if the code models the phenomenon (=YES), and mark '-' if it is not modelled (=NO)
- Some of the boxes need more details; short descriptions, continue in the text section of the deliverable report if necessary
- Fission product behaviour is separated into LOCA and SGTR, as the phenomena in these two are different regarding FP behaviour

Due to the large size of the table for integral system codes / thermal hydraulics codes, it is divided below into four tables: Table 3.2a-1 and Table 3.2a-2 has the first set of codes, and Table 3.2b-1 and Table 3.2b-2 has the second set.

Complementing the code descriptions (Section 2), the model comparison tables help to achieve an understanding on the foundations and the current capabilities of each of the applied code, e.g.:

Applied fuel behaviour codes…
→ being 0-, 1-, 1.5-, or 2.5-dimensional
→ only four out of twelve codes have some models for leaking fuel rods
→ only TRANSURANUS has an FGR model specifically for LOCAs

Applied system and TH codes…
→ several differences in modelling of fission product behaviour in LOCA conditions
→ only ATHLET-CD, ASTEC and MELCOR model the fission product behaviour in SGTR conditions

Table 3.1. Fuel performance and radionuclides behaviour modelling.

		Numerical structure of the code			Mechanical and thermal modelling																					Cladding failure model							Fuel chemistry and microstructure, fission product behaviour including fission gases																Leaking fuel rod simulation capabilities										
					Pellet											Pellet-cladding contact		Cladding							Coolant																																							
Code	Code version used in R2CA	Code dimensioning (1.5D, 2D, 3D)	Discretization: Finite-element (FE) or finite-difference (FD)	Mechanical / Thermal	Thermal expansion	Gaseous swelling	Rigid pellet approximation is used	Fuel creep: Irradiation creep	Fuel creep: Thermal creep	Pellet cracks or cracking are modelled	Pellet fragment axial relocation model	Fuel specific heat capacity is a function of	Fuel thermal conductivity is a function of	Formation of high burnup structure at the pellet rim is taken into account	Pellet-cladding friction when the gap is closed (sliding)	Sticking option is used when the gap is closed (no slipping between pellet and cladding)	Thin cladding wall approximation is used	Axisymmetric cladding deformation: Irradiation creep	Axisymmetric cladding deformation: Cladding creep	Above yield stress, the plastic strain is rate dependent: axially	Above yield stress, the plastic strain is rate dependent: circumferentially	Oxide layer thermal conductivity is considered	Subchannel thermal-hydraulics is modelled	Stress based	Strain based	Critical Strain Energy Density (CSED)	Fracture mechanics approach	Cumulative Damage Index (CDI)	Some other model, which?	No cladding failure prediction available	FGR is given by: correlation(s)	FGR is given by: mechanistic model(s)	FGR is given by: other approach	There is a FGR model specifically for LOCAs	Separation of fission gases into intergranular, intragranular and pore gas	Fission product release is correlated with FGR	There is a model of fission product behavior that accounts for: fission product diffusion	There is a model of fission product behavior that accounts for: interaction with micro-structure (bubbles, dislocations)	There is a model of fission product behavior that accounts for: formation of chemical compounds	There is a model for: stoichiometric deviation	There is a model for: change in average U/O ratio	There is a model for: stoichiometric deviation that accounts for: oxygen radial redistribution in thermal gradient	Activity release from the pellet into the free volume of fuel rod	Steady state activity release from fuel rod	Transient activity release from fuel rod (spiking)	Hydrogen production and accumulation inside of leaking rod	Hydrogen uptake by Zr cladding	Formation of secondary defect in the leaking rod	Leaching of pellets by coolant
DYN3D	v.3.3	1D	FD	FD	X	-	-	-	-	-	-	T	T,B	-	-	X	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FRAPCON	4	1.5	FD (Alternative FEA mechanical model, not validated)	FD	X	X	X	-	-	-	-	Temperature, composition, molten fraction, O/M ratio	Temperature, density, O/M ratio, plutonium content, burnup	X	X (Only in the alternative FEA mechanical model)	X	X	X	X	-	X	X	-	-	-	-	-	-	X (The output shows an uniform strain which may be used as a limit to compare)	-	-	X (Resolution of the modified Forsberg-Massih model, which depends on parameters that are based on empirical correlations)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FUROM	2.2	1.5	FD	FD	X	-	X	-	-	-	-	-	T, BU, porosity, Gd content	X	X	X (Sliding or sticking are both possible options, the choice has to be made in the input)	-	X	X	X	-	-	X	X	-	-	-	-	X	-	-	X	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
SHOWBIZ	1.0	1.5D,	FE	FD	No pellet												-	x	-	x	-	-	X	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	X	-	-	-	-	-	-	-	-	-	-
TRANSURANUS	v1m3j19	1.5D	FD	FD	X	X	X	X	X	X	-	T,B	T,B	X	X	-	X	-	X	X	X	-	X	X	X	X	X	-	X	-	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
DRACCAR	V3.0.1	2.5D	alternative mechanical model	FV	X	-	-	-	-	-	X	T, porosity, composition	T, porosity, composition	-	-	X	X	-	-	X	X	-	-	X	X	X	X	-	X (Critical temperature based rupture model)	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FRAPTRAN	1.5 (VTT); 2.0 (CIEMAT, EK)	1.5	FD (Alternative FEA mechanical model, not validated)	FD	X	-	X	-	-	-	-	Temperature, composition, molten fraction, O/M ratio	Temperature, density, O/M ratio, plutonium content, burnup	X	X (Only in the alternative FEA mechanical model)	X	X (In the alternative FEA mechanical model the cladding is nodalized)	X	-	-	X	X	-	X	X	X	X	X	-	X	-	X (Based on temperature thresholds)	-	X	X	X	X	X	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
MFPR-F	1.0	1D	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
TSKGO	n.a.	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	X	X	X	X	-	X
RING	n.a.	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	X	X	-	-	-	-
AC²: ATHLET-CD	AC² version 2019, ATHLET-CD 3.2	1D	FD	FD	X	-	-	-	-	-	-	T	T	-	-	X	X	X	-	X	?? (should be clarified)	-	X	X	-	X (user selects the failure criterion from four options, see Section 2.13.1.2)	X	-	-	-	X	-	-	X	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ASTEC: ELSA	v2.1	0D	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-

Table 3.2a-1. Integral system codes and thermal hydraulics codes (table continues in the next page).

Code	Code version used in R2CA	Numerical structure of the code												Thermal hydraulic models					Core region									
		Time-integration	semi-implicit	fully-implicit	Discretisation	Finite-element	Finite-difference (FD)	Other, which?	Variable arrangement	staggered	collocated	Other features?	Flow model: drift-flux, two-fluid, three-field, etc.	3D module available for RPV	Containment model available or to be coupled	Models available for fission product transport	Description of flow regimes taken into account	Any other important features, e.g. regarding uncertainties?	Neutron kinetics	1D	3D	point kinetics	Type of TH-neutronics coupling	Method for determining the hot rod maximum temperature	Gap conductance model	Fuel rod cladding deformation models	Decay heat model	Any other important features?
CATHARE		x					x		x				three fields	x	x		x					x		No internal model; given by other coupled mode	constant or computed	No internal model; given by other coupled mode	imposed	
GENFLO	2.3	x	-	-	-	-	finite difference for momentum and mass equations	donor cell differencing scheme for energy equations	x	-	-	-	two energy and mass equations, one momentum equation, drift-flux phase separation	Parallel channel modelling in the core with 1-D thermohydraulics	-	-	single-phase liquid/steam, bubble or slug flow, annular/inverted annular flow, dispersed droplet flow	-	-	-	-	x	-	Simple fuel rod model that calculates the fuel rod thermal behaviour	Fixed gap conductivity value given via input or from fuel performance code in coupled mode	No internal model; given by the fuel performance code in coupled mode	Decay heat power is given as an input	
RELAP5	Mod 2.5 (TRACTEBEL, required for licensing calculation in Belgium)	x	-	-	-	-	x	-	x	-	-	-	Non-homogeneous and non-equilibrium model for two-phase system (6 equations for phasic mass, momentum and energy + non-condensable and boron mass conservation equations)	-	-	-	Vertical: - pre-CHF: bubbly, slug and annular mist, stratified - post-CHF: inverted annular, inverted slug and mist Horizontal: similar to vertical pre-CHF - pre-CHF as vertical - no post-CHF regime	-	-	-	-	-	2 models available: - separable model: nonlinear feedback effects from moderator density and fuel temperature changes and linear feedback effects from moderator temperature changes, Doppler reactivity, boron concentration - tabular model: nonlinear feedback effects from moderator density, fuel temperature changes, moderator temperature and Boron feedback via four-dimensional table	Determined by the modeling approach	dynamic gap conductance model defines an effective gap conductivity based on a simplified deformation model generated from FRAP-T6: - fuel-to-cladding radiation heat transfer is neglected; - mid-range gap conductivity that means the gap conductivity is about the same order as that of metals - direct contact of fuel and cladding is not considered	no cladding ballooning effect included	Model based on 1979 ANS Standard for decay heat power in light water reactor is available	-
	Mod 3.2 and Mod 3.3 (SSTC)																											
RELAP5-3D		x	-	-	-	-	x	-	x	-	-	-	See Relap5	x	I	X (simplified model available)	See Relap5	-	-	Internal coupled to Nestle	x	Internal coupling	Hot rod needs to be modelled	x	-	See Relap	x

Table 3.2a-2. Integral system codes and thermal hydraulics codes (table continued from the previous page).

Correlations and methods

Code	Chocked flow models applied in LOCA & SGTR	Short description of reflood modeling approach	Critical heat flux correlation for rod bundles	CCFL correlation & where applied	Forced convection heat transfer	Wall-to-fluid heat transfer correlations	Film boiling heat transfer	Interfacial drag correlations	Spacer grid modelling (heat transfer, hydraulic resistance)
CATHARE	-	PSCHIT model (local refinement of meshing)	-	-	Dittus-Boelter	laminar, forced, bucleate boiling, transition, film boiling	-	-	pressure loss only
GENFLO	-	All heat transfer modes exist over the whole post-dryout regime. The liquid volumetric fraction is the main parameter defining the strength of the heat transfer mode.	Simplified fit to typical critical heat flux correlations, see the table in the code description	Described with Zuber-Findlay drift flux model	Dittus-Boelter	Dittus-Boelter for pre-saturation, fitted models for nucleate boiling, transition boiling and film boiling, cf. Table in code description	h=200(1-α)D, where D=constant with recommended range 0.05 – 10.0, and nominal value of 0.2; α=void fraction	-	-
RELAP5	yes - Ransom-Trapp model	two-dimensional conduction scheme is used in reflood model - similar to COBRA-TF (but model obviously not used for SGTR cases)	Biasi for High Flow CHF correlation (mass flux > 200 kg/m²/s) Modified Zuber CHF correlation (mass flux < 100 kg/m²/s) If mass flux is in between 100 and 200 kg/m²/s, a linear interpolation with respect to mass fux is used	no CCFL correlation (no f flag available)	Dittus-Boelter correlation used for single phase Wall to Liquid, Liquid to Wall, Vapor to Wall, or Wall to Vapor	Dittus-Boelter correlation used for single phase Wall to Liquid, Liquid to Wall, Vapor to Wall, or Wall to Vapor	Modified Bromley-Pomeranz, Breen and Westwater	evaluation of the drag coefficient with Ishii and Chawla and interfacial area with Ishii and Mishima	-
	Ransom-Trapp model; Modified Henry-Fauske model	two-dimensional conduction with code-controlled fine mesh adjustment. Reflood-specific adjustments to wall and interfacial heat transfer, and interfacial drag calculation for bundle and non-bundle structures	1986 AECL-UO CHF lookup table or PG-CHF (Rez) correlations for high flow CHF correlation (mass flux > 200 kg/m²/s) Modified Zuber CHF correlation (mass flux < 100 kg/m²/s) If mass flux is in between 100 and 200 kg/m²/s, a linear interpolation with respect to mass fux is used	Kutateladze, Wallis or their weighted combination form of CCFL	Dittus-Boelter correlation, Innayatov turbulent flow multiplier for vertical bundles with parallel flow	Natural convection: Churchill-Chu correlation, McAdams Forced convection: Dittus-Boelter+Innayatov coefficient for vertical bundles Nucleate and transition boiling: Chen correlation Film boiling: Modified Bromley correlation	Modified Bromley correlation	drift flux model for vertical bubbly and vertical slug flow; drag coefficient model (Ishii and Chawla) for other modes	hydraulic resistance as form loss coefficients; grid spacer factor in CHF calculation with 1986 AECL-UO lookup table
RELAP5-3D	Ransom Trapp/Henry Fauske	Possibility to enable 2D heat transfer during reflood	Groeneveld Look-up tables	Bankoff, Wallis Kutateladze	See Relap5	See Relap5	See Relap5	See Relap5	Spacer grid position used for CHF calculation

Fission Products - LOCA conditions

Code	Fission gases are considered	Volatile FP are considered	Semi-volatile FP are considered	Model for FP release from fuel	Speciation of FP released from fuel	Fission product transport in primary circuit							Fission product behavior in containment															
						Transport in gaseous phase	Chemistry in gasous phase	Evaporation/condensation on walls	Evaporation/condensation on aerosols	Aerosol transport	Aerosol deposition	Aerosol resuspension	Model for FP release from fuel	Speciation of FP released from fuel	Chemistry in gasous phase	Radiochemistry in gaseous phase	Evaporation/condensation on walls	Adsorption/desorption on painted walls	Radiochemistry on painted walls	Aerosol deposition	Aerosol washing	Aerosol radiolysis	Aerosol spray capture	Chemistry in liquid phase	Radiochemistry in liquid phase	pH effect in liquid phase	Iodine chemistry in gas phase	Iodine chemistry in liquid phase
CATHARE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GENFLO	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
RELAP5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
RELAP5-3D	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Fission Products - SGTR conditions

Code	Fission gases are considered	Volatile FP are considered	Semi-volatile FP are considered	Model for FP release from fuel	Speciation of FP released from fuel	Fission product transport in primary circuit			Fission product transport in secondary circuit				
						Transport in liquid phase	Chemistry in liquid phase	Wall deposition from liquid phase	Model for FP partition at SG breach (flashing, carry-over…)	Retention in SG liquid phase	Retention in SG separator-dryer	Transport in gaseous phase	Chemistry in gasous phase
CATHARE	-	-	-	-	-	-	-	-	-	-	-	-	-
GENFLO	-	-	-	-	-	-	-	-	-	-	-	-	-
RELAP5	-	-	-	-	-	-	-	-	-	-	-	Can be simulated by user as noncondensable gas	-
	-	-	-	-	-	-	-	-	-	-	-		-
RELAP5-3D	-	-	-	-	-	x	-	-	-	-	-	x	-

Table 3.2b-1. Integral system codes and thermal hydraulics codes (table continued from the previous page).

Code	Code version used in R2CA	Numerical structure of the code								Thermal hydraulic models					Core region										
		Time-integration	semi-implicit	fully-implicit	Finite-element	Finite-difference (FD)	Other, which?	staggered	co located	Variable arrangement	Other features?	Flow model: drift-flux, two-fluid, three-field, etc.	3D module available for RPV	Containment model available or to be coupled	Models available for fission product transport	Description of flow regimes taken into account	Any other important features, e.g. regarding uncertainties?	Neutron kinetics			Type of TH-neutronics coupling	Method for determining the hot rod maximum temperature	Gap conductance model	Fuel rod cladding deformation models	Decay heat model	Any other important features?
																		1D	3D	point kinetics						
MELCOR	v2.2_15254 (CIEMAT)	X (Bel V) A semi-implicit (finite-cell) formulation of the governing equations is used to permit timesteps greater than the acoustic Courant limit (CIEMAT)	-							-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ASTEC	V2.2	-	X			FV				Control Volume/flow path approach (CIEMAT)	-	By default: drift-flux Two-fluid (6 equations) available on user option	-	-	-	Stratified, dispersed flow and mist flow, droplet entrainment	-	-	-	-	-	-	-	-	-
APROS		X (implicit Euler)	X	-	X	-	X	X	-	X	-	X	X	X	X	X	-	X	X	X	-	-	-	-	-	-
COCOSYS	V2.4v5	I	X	I	X	I	I	X	X	X	-	X	I	X	X	X	X	I	I	I	I	I	I	I	I	I
AC^2: ATHLET-CD	3.2	I	X			I		X		two ph. systems available: - 5eq. Model (mix. Momentum eq.) - 6eq. Model (two fluid model) full range drift-flux model		COCOSYS (or simplified CONDRU model)			X		-mixture level model -boron transport model -model for non condensables	X (limited to simulation of single rod or single group of rods)	I	(only by coupling to external codes such as DYN3D)	X	-Reactivity effects: fuel temperature, coolant moderator density, boron concentration, void fraction (soon to be tested (to author's knowledge). However, ORESTE/PISO for decay heat calculation cannot be coupled with neutron kinetics module. For complex accident scenarios investigated (severe) accidents (such as long-term SBO, or a LOCA with long term unavailability of safety systems) where neutron kinetics is not used. Calculations are started with constant reactor power, SCRAM (reduction of fission power) is given by tabular time dependent values.	hot rod can be modelled separately as HCO with high power	X	-	-
AC^2: ATHLET	3.2	I	X	I	I	FV	I	X	I	pseudo 3D	I	I	I	I	I	X	X (? To be checked, never tested by author)	I	(only by coupling to external codes such as DYN3D)	X	in general the same neutronics model as for ATHLET (1D or point kinetics, COCOSYS (or simplified CONDRU model) however, ORESTE/PISO for decay heat calculation cannot be coupled with neutron kinetics module. For complex accident scenarios investigated (severe) accidents (such as long-term SBO, or a LOCA with long term unavailability of safety systems) where neutron kinetics is not used. Calculations are started with constant reactor power, SCRAM (reduction of fission power) is given by tabular time dependent values.	-Reactivity effects: fuel temperature, coolant moderator density, boron concentration, void fraction (soon to be tested (to author's knowledge). However, ORESTE/PISO for decay heat calculation cannot be coupled with neutron kinetics module. For complex accident scenarios investigated (severe) accidents (such as long-term SBO, or a LOCA with long term unavailability of safety systems) where neutron kinetics is not used. Calculations are started with constant reactor power, SCRAM (reduction of fission power) is given by tabular time dependent values.	hot rod can be modelled separately as hot rod object with high power	X	X	I	-	-
DYN3D	v.3.3	-	-	-	-	X	-	-	-	-	-	2-phase fluid	-	-	-	X	-	3D	-	-	-	-	-	-	-

Table 3.2b-2. Integral system codes and thermal hydraulics codes (table continued from the previous page).

Group	Subgroup	Code	AC^2: ATHLET	AC^2: ATHLET-CD	AC^2: COCOSYS	APROS	ASTEC	MELCOR	DYN3D
Correlations and methods		Chocked flow models applied in LOCA & SGTR	X (four different models available: sonic velocity model, HEM model, Moody model, CDR1D model (defaul))		-	Moody & Henry-Fauske	Gros d'Aillon correlation from CATHARE [Geffraye, Geneviève, et al CATHARE 2 V2.5 2: A single version for various applications Nuclear Engineering and Design 241 (2011) 4456–4463]	X	-
		Short description of reflood modeling approach	2 approaches available: 'spontaneous' local rewetting model and quench front model with Semeria/Martinet and Yamanouchi correlation for quench front velocity		-	Adaptive fine meshing of the heat structures + reflood-specific closure laws for wall heat transfer and interfacial phenomena.	Quench front detection assuming a step-shape T profile from Tsat to Tfilmboiling Specific heat transfer coefficient (user-defined) applied above the quench front to simulate droplet projection	X	-
		Critical heat flux correlation for rod bundles	10 different correlations implemented, e.g. Westinghouse W-3, Hench-Levy, Israel-Casterline-Matzner or Biasi for high pressure (default = minimum value of these four correlations), Zuber for low pressure, Gidropress for WWER, Osmachkin for RBMK + user-defined correlations via plugin-approach		-	Selectable from: Groenevel LUT, Biasi, Zuber-Griffith, Smolin, Bezrukov, etcc.	Zuber's correlation for pool boiling with the correction on liquid subcooling due to Ivey and Morris [H.J. Ivey and D.J. Morris. On the relevance of the vapour-liquid exchange mechanism for subcooled boiling heat transfer at high pressure. Rept AEEW-R137, UKAEA, Winfrith, 1962.]	X	IAE-4, OKB-2, Pernica
		CCFL correlation & where applied	part of drift-flux model (applied in each junction), special models for cold leg injection and hot leg injection		-	Kutateladze-type CCFL correlation specified by the user at user-selectable locations (typically upper tie plate & downcomer)	No CCFL	X (BEL V); The stratified CCFL model is intended to model stratified counter current flow of gases in a flow path (CIEMAT)	-
		Forced convection heat transfer	Dittus-Boelter for single phase, since version 3.1 new bundle factor according to Inayatov		X	Dittus-Boelter or Gnielinski correlation	Liquid: Dittus-Boelter correlation corrected by a Chen correlation (from CATHARE) Gas: Dittus-Boelter correlation	X	X
		Wall-to-fluid heat transfer correlations	Dittus-Boelter correlation		X	Forced & natural convection + Thom for nucleate boiling + Berenson for film boiling. Interpolation between Thom and Berenson for transition boiling.	Below saturation, maximum between natural (several correlations) and forced convection, in laminar and turbulent regimes. Condensation, nucleate boiling, film boiling, radiation.	X	one–phase liquid (laminar/turbulent natural or forced convection) and developed boiling heat transfer
		Film boiling heat transfer	Several correlations implemented: Modified Dougall-Rohsenow; Groeneveld 5.9; Condie-Bengston IV		-	Modified Berenson correlation	Berenson correlation (P.J. Berenson. Film boiling heat transfer from a horizontal surface. Journal of Heat Transfer, 83(3):351–358, 1961.).	X	X
		Interfacial drag correlations			X	Bestion correlation for bubbly/slug/churn flows in pipes and bundles. IVO-correlation for VVER rod bundles. Correlation for mist/droplet flow.	From Bestion et al (Nuclear Engineering and Design 124 (1990) 229-245)	X	-
		Spacer grid modelling (heat transfer, hydraulic resistance)	hydraulic resistance as form loss coefficients	hydraulic resistance as form loss coefficients	-	Flow area reduction & hydraulic loss specified by the user. Correlation for droplet breaking effect.	No specific heat transfer correlation (same laws as rods). Increase regular pressure losses by reducing hydraulic diameter. It is recommended to introduce user-defined singular pressure losses (not included in PWR900-LIKE input deck).	X	hydraulic resistance
Fission Products - LOCA conditions		Fission gases are considered	-	X	X	X	X	X	-
		Volatile FP are considered	-	X	X	X	X	X	-
		Semi-volatile FP are considered	-	X	-	X	X	X	-
		Model for FP release from fuel	-	Temperature dependent Arhenius equations + function of partial pressures for some elements Two options: Release if specified rod temperature is exceeded or burst according to rod deformation model	-	If the max. cladding temperature of a core channel reaches its limit (given by user) cladding is assumed to be failed → temperature dependent Arrhenius equation determines the FP release. More detail in the code description.	X	X	-
		Speciation of FP released from fuel	-	Release of up to 24 element groups, decay heat of released FPs is calculated	-	Chemical speciation is modelled but radioactive decay is taken into account.	-	X (classes)	-
	Fission product transport in primary circuit	Transport in gaseous phase	-	X	-	X	X	X	-
		Chemistry in gasous phase	-	X	-	-	X	-	-
		Evaporation/condensation on walls	-	X	-	X	X	X	-
		Evaporation/condensation on aerosols	-	X	-	-	X	X	-
		Aerosol transport	-	X	-	X	X	X	-
		Aerosol deposition	-	X	-	X	X	X	-
		Aerosol resuspension	-	X	-	X	X	X	-
	Fission product behavior in containment	Model for FP release from fuel	-	-	-	If the max. cladding temperature of a core channel reaches its limit (given by user) cladding is assumed to be failed → temperature dependent Arrhenius equation determines the FP release. More detail in the code description.	X	X	-
		Speciation of FP released from fuel	-	-	-	Chemical speciation is modelled but radioactive decay is taken into account.	-	X (classes)	-
		Chemistry in gasous phase	-	-	X	-	X	-	-
		Radiochemistry in gaseous phase	-	-	X	-	X	-	-
		Evaporation/condensation on walls	-	-	X	X	X	X	-
		Adsorption/desorption on painted walls	-	-	X	-	X	X	-
		Radiochemistry on painted walls	-	-	X	-	X	-	-
		Aerosol deposition	-	-	X	X	X	X	-
		Aerosol washing	-	-	X	-	X	X	-
		Aerosol radiolysis	-	-	X	-	X	-	-
		Aerosol spray capture	-	-	X	X	X	-	-
		Chemistry in liquid phase	-	-	X	-	X	-	-
		Radiochemistry in liquid phase	-	-	X	-	X	-	-
		pH effect in liquid phase	-	-	X	pH of coolant is considered in FIPROMO	X	X	-
		Iodine chemistry in gas phase	-	-	X	-	X	-	-
		Iodine chemistry in liquid phase	-	-	X	-	X	X	-
Fission Products - SGTR conditions		Fission gases are considered	-	X	-	-	X	X	-
		Volatile FP are considered	-	X	-	-	X	X	-
		Semi-volatile FP are considered	-	X	-	-	X	X	-
		Model for FP release from fuel	-	Temperature dependent Arhenius equations + function of partial pressures for some elements Two options: Release if specified rod temperature is exceeded or burst according to rod deformation model	-	-	X	X	-
		Speciation of FP released from fuel	-	Release of up to 24 element groups, decay heat of released FPs is calculated	-	-	-	X (classes)	-
	Fission product transport in primary circuit	Transport in liquid phase	-	X (Details for modelling of SGTR should be confirmed by the code owner GRS. Within R2CA, ATHLET-CD will be used only for LOCA)	-	-	X	X	-
		Chemistry in liquid phase	-	X	-	-	X	-	-
		Wall deposition from liquid phase	-	X	-	-	X	X	-
	Fission product transport in secondary circuit	Model for FP partition at SG breach (flashing, carry-over…)	-	X	-	-	X	-	-
		Retention in SG liquid phase	-	X	-	-	X	X	-
		Retention in SG separator-dryer	-	-	-	-	X	X	-
		Transport in gaseous phase	-	X	-	-	X	X	-
		Chemistry in gasous phase	-	X	-	-	X	-	-

4. Summary of the development needs

Major developments are planned along the R2CA project at different modelling levels, from specific phenomena to scenario nodalization going through complex processes, like FP transport and chemistry. Then the development needs are grouped in the following four sections:

5.2.1. Clad modelling
5.2.2. Fuel and FP modelling
5.2.3. Codes coupling
5.2.4. Whole core modelling and nodalization

4.1 Cladding modelling

IRSN identified specific developments to model the formation of secondary hydride region of failed fuel rods, during normal operating conditions, in SHOWBIZ code. In particular, a 1D fluid channel will be implemented, along the R2CA project, to take into account the gas transport in the fuel-cladding gap and subsequent oxidation and hydrogen pickup at the inner surface of the clad. H2 diffusion in the cladding thickness and eventually the formation of blister will be also implemented. In addition, failure criteria for hydrided cladding will be defined.

JRC will be involved in the development of models for the hydrogen uptake under DBA condition and redistributing in the cladding for the TRANSURANUS code. Model for radial hydrogen redistribution in the cladding will also be done within a TRANSURANUS bilateral licence agreement, followed by JRC's independent testing. New models will be implemented by JRC to take into account the effect of hydrogen content on the creep behaviour of Zircaloy-4 claddings. ENEA will extend the applicability of TRANSURANUS to the simulation of a LOCA with fuel assemblies equipped by M5 claddings (effects of the hydrogen uptake on the M5 cladding material properties and on cladding burst models relevant for LOCA). UJV will enhance the capability of TRANSURANUS by implementing models for the transport of the gas in the rod before and after burst. Such models have impact on the prediction of cladding ballooning and on the location and extent of the secondary hydriding region.

The development of DRACCAR platform is planned by IRSN to allow, in a single LOCA simulation, the detailed description of the thermal-mechanical behaviour of a group of rods, at the scale of a fuel assembly, by taking into account the interaction with neighbouring rods, modelled using a weighted averaged single rod approach inside each homogenized cells of a coarser meshing. A high-performance numerical approach and specific verifications and validation of the interactions between the fine and coarse meshings with transition rules between scales, are required to obtain a consistent description of the whole core thermal-mechanical behaviour.

In relation to FRAPTRAN code, the LOCA cladding failure predictions will be improved by EK and VTT on the basis of the experimental database re-assessment on cladding failure, under LOCA conditions, planned in R2CA. In particular, re-assessment of cladding failure limits and plastic deformation model parameters in FRAPTRAN for E110 and E110G is planned by EK. CIEMAT plans to contribute to fuel rod modelling on two aspects: in-cladding secondary hydriding and cladding failure. As for the former, models for distribution and precipitation of secondary hydrogen uptake under operations conditions of defective fuel rods will be coupled with FRAPCON, so that cladding embrittlement will be better estimated. As for cladding failure, the cladding failure modelling in FRAPTRAN will be reviewed and, based on a re-assessment of the experiments made available in the project, an enhancement of the model or an alternate one might be proposed and implemented.

In relation to the TSKGO code, the hydrogen uptake model of E110 alloy will be updated by EK on the basis of new experimental data.

For ATHLET-CD, one of the codes of AC^2, possible improvements will be performed by HZDR in collaboration with the code developer GRS in relation to the:

- Current code limitations that allow to define only one set of fuel parameters in the input (e.g. gas gap pressure);

- Current missing dependence of gas gap pressure and other rod conditions on burnup.

In relation to the steady-state FRAPCON code, a model of hydrogen migration/precipitation of secondary hydrogen uptake under operations conditions of defective fuel rods will be coupled with FRAPCON by CIEMAT, so that cladding embrittlement will be better estimated.

4.2 Fuel and fission product modelling

In relation to RELAP5-3D and considering that radioactive decay cannot be modelled adequately with this code, it would be an important achievement for BOKU in the R2CA project if radioactive decay could be included into the model via an external device. RELAP5-3D has a very rough model for radionuclide transport. The user can specify for up to 99 radionuclides if they are transported in the liquid or steam phase of the default fluid. BOKU aims to write an external model to the RELAP5-3D radionuclide transport that would include radioactive decay. Even though the radio chemistry would still be missing, the precise thermal hydraulic modelling that RELAP5-3D is providing (compared to integral codes) would outweigh the shortcomings in DEC-A transients.

JRC plans to implement the ANS5.4 model for radioactive fission product release in TRANSURANUS. POLIMI targets to couple SCIANTIX (POLIMI's in-house fission gas behaviour module) with TRANSURANUS and to implement in SCIANTIX an updated version of the ANS5.4. In particular, instead of the present semi-empirical approach, the grain boundary coverage fraction defined in state-of-the-art mechanistic models for inert gas behaviour will be considered for modifying the ANS5.4. A model of high burnup structure formation and evolution will be also added in SCIANTIX. IRSN will extend the existing TRANSURANUS/MFPR-F coupled code allowing the activation of the HBS model of MFPR-F in the coupling. The coupling will be extended to oxidising conditions following cladding breach, provided that the oxygen potential in the gap can be derived from the model for axial gas evolution developed for failed fuel by UJV. UJV will also improve the modelling of the fuel temperature in failed rods. NINE will implement correlations from open literature into TRANSURANUS considering analytical models for the prediction of FGR from defective fuel.

In relation to MFPR-F code, for IRSN a model accounting for the mechanical process of fuel cracking under HBS pore over pressurization is required for a more mechanistic approach for estimating the FG and volatile FP release during LOCA transient. Thanks to recent developments, the MFPR-F code takes into accounts the formation and growth of HBS during irradiation, and the FP release during thermal transients. This model is already available in MFPR-F but it does not account for the effect of cladding restrain. The recent coupling of MFPR-F with the fuel performance code TRANSURANUS will address this issue. IRSN, along the R2CA project, will make the suitable adaptations so that the HBS model of MFPR-F can be activated in the coupled code. In addition, a model for fission gas gap releases during LOCA will be implemented in DRACCAR.

Finally, oxidation-induced FG releases occurring after cladding burst will also be addressed by IRSN through the coupled TRANSURANUS/MFPR-F code and the modelling of stoichiometric deviation in the fuel taking advantage of the new model of gas transport in failed rod which will be implemented in TRANSURANUS. The coupled TRANSURANUS/MFPR-F code will be used to calculate the transient release of iodine and the iodine spike within SGTR conditions.

In relation to Ring code, EK will update the transient model using new shutdown iodine spiking data from a VVER reactor.

Various development needs of APROS code have been identified by VTT but these developments are done outside the R2CA project. The development items include: improvement of Zr oxidation model to account for boron - stainless steel - zirconium interactions during core degradation; better estimation of structural material release, especially for tin from zircaloy cladding and for semi/low volatile FP release; improved description of gaseous iodine behaviour in the RCS taking into account the kinetics of iodine reactions in the primary system; development of in-vessel melt pool models (e.g. with Ag-In-Cd and oxidized SS); development of a model for FP aerosol agglomeration into larger particles; improvement of dose rate calculation taking into account the shielding effect of water on containment floor and, finally, expansion of chemistry libraries.

For IRSN, the modules of ASTEC code dealing with FP/SM release from the core, and iodine chemistry in the containment (in particular dose rate has to be evaluated in LOCA), are designed for severe accident conditions and they might need some reassessment for the more limited conditions of DBA along R2CA project. In the case of SGTR, the models for Iodine chemistry in the primary loops and the partition of iodine following the jet flashing at SGT breach have to be improved especially by a better assessment of the iodine chemical forms transported in the primary circuit. This will be not part of R2CA project.

In relation to MELCOR code, further development needs are identified by the MELCOR Peer Review in RCS deposition, chemical reactions with surface, and aqueous chemistry. Within R2CA, MELCOR code development is not foreseen, however the results of the MELCOR applications will be presented in the CSARP (Cooperative Severe Accident Research Program) framework [1]; then potential code development needs, if any, will be underlined. Therefore, if some development of the code will be implemented, the new release of MELCOR could be used in the R2CA project.

EDF intends to improve the modelling, already existing in the EDF version of the EPRI MAAP5 code, of FP transport from the primary circuit to the environment during SGTR analysis. This includes the implementation of enhanced correlations and the evaluation of this improvement. Iodine spiking impact on results should be analysed, see [3].

4.3 Coupling of codes

Coupling between GENFLO and the latest FRAPTRAN 2.0 (release 2016) version could be possible in the frame of R2CA, but VTT has yet to decide if it is worthwhile considering that the U.S. NRC's new FAST code is set to replace both FRAPCON and FRAPTRAN in the near future.

In relation to RELAP5, the calculated data can be used by SSTC and UJV (or UJV may use ATHLET instead of RELAP5) as an input for TRANSURANUS.

In relation to TRANSURANUS, it will be coupled by POLIMI with the in-house fission gas behaviour module SCIANTIX, before mentioned. The coupling between the MFPR-F code and the TRANSURANUS code will be extended by IRSN, as previously underlined.

IRSN will study the possibility to couple DRACCAR to SOPHAEROS module of ASTEC through ODESSA in a common platform to assess the transport of the FPs in the primary circuit, in the containment and finally the Radiological Consequences.

Development of data exchange between JRodos and other codes (namely AC^2) is envisaged by UJV. UJV intends to implement the computational chain consisting of TRANSURANUS, ATHLET-CD and JRODOS, and develop a special software tool for data transfer between ATHLET-CD and JRODOS, see [3].

In relation to FEMAXI code, a calculation procedure for using FEMAXI results with ASTEC should be implemented by LEI if the preliminary plan to use a calculation chain RELAP5 (alternatively: ASTEC) → FEMAXI → ASTEC for the LOCA studies at LEI is carried out. However, it is likely that FEMAXI is replaced by TRANSURANUS in the calculation chain.

In relation to FUROM code, no code development is foreseen in the framework of the R2CA project, as it only provides input data for the codes that simulate transient fuel behaviour.

4.4 Whole core modelling and nodalization

In the application of ATHLET-CD, HZDR plans to apply a new approach of the core modelling and nodalization: in particular the core can be sub-divided into a larger number of sections (also azimuthal subdivision). Furthermore, the current input deck of the Generic Konvoi PWR model will be updated in such a way that flow distribution during blow-down and reflood phase of the LOCA transient is simulated more accurately.

In the frame of R2CA, DRACCAR capabilities will be extended to the description of the whole core coupled to reactor primary and secondary loops. It means that core domain will not be limited to a weighted single equivalent fuel assembly or only to average weighted rods located in T/H core rings. This approach will mix modelling scales with fined assembly description at sub-channel scale as well as coarser meshing using lumped volume and equivalent weighted rods to depict other part of the core. Both scales will be managed in a single simulation proposing the whole core response to LOCA. This work should lead to propose new type of applications able to take into account more in depth the behaviour of some fuel assemblies and their interaction with the rest of the core. In a further step, the core domain will be included in a whole reactor circuit simulation (RPV, primary and secondary loops), see [2].

UJV will further develop the statistical approach which is currently used for the core-wide LOCA analysis of the Czech NPPs in order to provide more robust estimate of the number of the failed rods. The approach will be elaborated using ATHLET – TRANSURANUS or RELAP5 – TRANSURANUS sequence, see [2].

4.5 References

[1] Cooperative Severe Accident Research Program (CSARP), NUREG/BR-0524, USNRC, 2015, www.nrc.gov/docs/ML1532/ML15329A041.pdf
[2] V. Busser, A. Kecek, T. Taurines, A. Schubert, Detailed Program of Work for WP3, R2CA project report, draft version 21-02-2020
[3] Z. Hózer, L. Herranz, L. Luzzi, C. Leclere, Detailed Program of Work for WP4, R2CA project report, draft version 02-07-2020

5. Summary and conclusions

This report summarizes the modelling computer programmes used in the R2CA project for the simulation of LOCA and SGTR. A complete list of described codes is given in Table 1.1 (Section 1). The report helps to achieve an understanding on the current capabilities of each of the applied code by utilizing code descriptions (Section 2) and model comparison tables (Section 3). The report summarizes also the general development items for the codes as well as those intended to be addressed in the R2CA project (Section 4). Many codes will gain significant improvements for modelling the phenomena addressed in the project, while some of the codes are not improved but used in the development of radiological consequences evaluation methodologies. In the latter case, development items may rise during the project. The distinguished development items can be grouped as follows: 1) cladding modelling, 2) fuel and fission product modelling, 3) codes coupling, and 4) the whole core modelling and nodalization.