KIT reactor safety research for LWRs: Research lines, numerical tools, and prospects

V.H. Sanchez-Espinoza *, F. Gabrielli, U. Imke, K. Zhang, L. Mercatali, G. Huaccho, J. Duran, A. Campos, A. Stakhanova, O. Murat, A.K. Mercan, J. Etcheto, M. Steinbrück, J. Stuckert, S. Gabriel, S. Ottenburger, R. Stieglitz, W. Tromm

Karlsruhe Institute of Technology, Institute for Neutron Physics and Reactor Technology Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

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A B S T R A C T

This paper describes the main research lines of the Karlsruhe Institute of Technology (KIT) relevant to Light Water Reactors (LWR) that permit both the safety evaluation of different reactor designs and the prediction of the radiological source term including its impact in the case of hypothetical severe accidents. The numerical tools for core analysis, nuclear power plant analysis of design basis and severe accidents, and the estimation of the radioactive dispersions of fission products after a core meltdown accident are described and selected results are discussed. The analytical investigations at KIT are complemented by experimental investigations at two facilities, namely the COSMOS-H/-L and the QUENCH facilities devoted to safety-relevant Thermal-Hydraulic (TH) phenomena and in-vessel severe accident early-phase for different kinds of fuel rods including Accident Tolerant Fuel (ATF). These data are crucial for the validation of the numerical tools used for safety demonstration. The paper is complemented by a brief description of the in-house tools under development for improved core/plant analysis based on the multi-physics/-scale coupling methodologies, where the in-house tools are combined with external system TH, Monte Carlo, and thermo-mechanic code to increase the prediction accuracy of the core/plant behaviour under stationary and accidental conditions. Selected results are presented and discussed. It can be stated that the long-lasting safety research activities at KIT devoted to LWR led to the development of a computation route combining external with in-house codes that is very much appropriate for safety evaluations and risk assessment; it includes unique multi-physics/-scale coupled tools for improved core and plant analysis of different reactor designs, e.g. PWR, VVER, BWR, SMR, and research reactors.

1. Introduction

After the Fukushima accident, the German government decided to terminate the use of nuclear energy for electricity production by continuously shutting down the 19 Nuclear Power Plants (NPP) until April 2023. As a consequence, the research programs of the Helmholtz Association (HGF) were adapted to account for the new German conditions within Europe. Apart from the identification of the sites for final disposal of the waste, an important and increasing activity is the intermediate storage and the decommissioning of NPPs as well as the regulatory tasks related to the research reactors under operation. These activities require expertise in radiation protection, the behavior of irradiated fuel, neutronics for the prediction of the nuclide inventory in the burnt fuel deposited in the intermediate storage facilities together with the estimation of the residual heat generated by the radioactive decay of the fission products and minor actinides. For the optimal planning of the decommissioning from the economic and radiation protection point of view, expertise in different fields such as nuclear engineering, reactor physics, radiation protection, and reactor safety in the regulators, operators, and different industries involved in such activities e.g. the proper estimation of the activation and contamination of key-components of an NPP. Moreover, around Germany more than 100 NPPs of different designs (Russian and Western) are in operation and a considerable number of NPPs are under planning. Considering that a nuclear accident with a large release of fission products takes place in a specific country but the dispersion of the released fission products does not stop in country borders. Instead, they spread out according to the actual local weather conditions and hence it is of primordial and

* Corresponding author.
E-mail address: victor.sanchez@kit.edu (V.H. Sanchez-Espinoza).

strategic importance that Germany keeps expertise for the own assessment of the radiological risks expected in Germany after a hypothetical severe accident with core melt that may occur in the neighbor country to undertake the timely countermeasures to protect the population. Knowing that the accurate estimation of the radiological risks after a severe accident in an NPP depends on the radionuclide inventory, its burnup, the design peculiarities of the NPP, and all the chemo-physical phenomena taking place during the evolution of a severe accident in the reactor core, the primary/secondary circuit and the containment that will determine the time and mode of failure of the safety barriers, it is of paramount importance for Germany to keep the expertise on relevant nuclear engineering related fields and continue with the improvement, validation, and application of the respective numerical simulation tools. In Fig. 1, a schematic representation of a Pressurized Light Water Reactor (PWR) is shown, where both the key-phenomena within the plant and the release of the fission product after the failure of the safety barriers – the last barrier is the containment- can be observed.

In line with the research program of the HGF and the 7th energy research program of Germany, the NUSAFE program at the Karlsruhe Institute of Technology (KIT) is deeply engaged in the development, validation, and application of the key numerical tools needed for the safety assessment of different NPP designs needed for the estimation of the radiological risk after a severe accident in any NPP around Germany and elsewhere. It is worth mentioning that numerical simulation tools are strongly used by regulators and technical support organizations for safety and risk assessment. Hence, they must reflect the state-of-the-art in science and technology. Consequently, these tools are under continuous improvements to account for the specificities of the different NPP-designs and the advances in nuclear technology reflected for example in new core loading of Light Water Reactor (LWR) Gen-II/-III and the Small Modular Reactors (SMR) characterized by increased burn-ups and high heterogeneity (Chanaron et al., 2015; Gaston et al., 2009; Palmtag et al., 2014). For a long time, best-estimate Thermal-Hydraulic (TH) codes with point or 1D kinetics have been used in the nuclear industry and by regulators. Nowadays, 3D neutron kinetics models based on the neutron diffusion approximation are mature and in extensive use, where the core is subdivided into many 3D nodes (e.g. 20 axial nodes and 1 radial node per fuel assembly) and the influence of the TH on the neutronics is taken into account via homogenized and condensed cross sections. To better face these challenges, KIT is developing different multi-physics coupled approaches that combine different neutronic deterministic / Monte Carlo transport codes with subchannel TH codes; in some cases also with thermo-mechanic codes for better description of the fuel behavior under irradiated conditions. The increased role of the radial reflectors of the SMR cores asks for more sophisticated methods. Here the Monte Carlo methods are a promising alternative. On the other hand, new reactor designs, e.g. water-cooled SMR are characterized by integrated Reactor Pressure Vessels (RPV), where different components, such as main coolant pumps, heat exchangers, pressurizer and in some cases flow mixer promoters, which disturb the 3D flow patterns inside the RPV. For such conditions, 1D TH system codes are no longer appropriate. To better describe the coolant behavior within the core and reactor pressure vessel in case of transients with local power distortions, the combination of 3D system TH, subchannel, and Computational Fluid Dynamic (CFD) codes instead of the 1D parallel channel approach of system TH codes is promising. Following worldwide trends, KIT is devoted to the development of multi-scale TH-coupled codes based on domain decomposition/ overlapping approaches and methodologies such as the External Communication Interface (ECI) and Interface for Code Coupling (ICoCo).

For the prediction of the overall risk that may arise from hypothetical severe accidents in NPPs of different designs under operation around Germany, KIT is developing a complete simulation chain of numerical tools based on in-house and external codes. They cover depletion codes for the estimation of the radionuclide core inventory at any operational time, integral severe accident codes for the prediction of all involved accident phenomena in the core, primary/secondary circuits, and the containment when fission products are released in the core and transported to the containment. The estimation of the radiological source term is an important pre-step to finally predict the radiological impact around the NPP after the accident using radionuclide dispersion tools based on which appropriate countermeasures can be undertaken by the emergency teams.

Last but not least, the role of methods and tools for the quantification of the embedded uncertainties of numerical tools is increasing in nuclear engineering for a best-estimate prediction of safety margins. Hence, KIT is developing its tools for these purposes, which can be used to quantify the uncertainties and sensitivities as well as their propagation from the

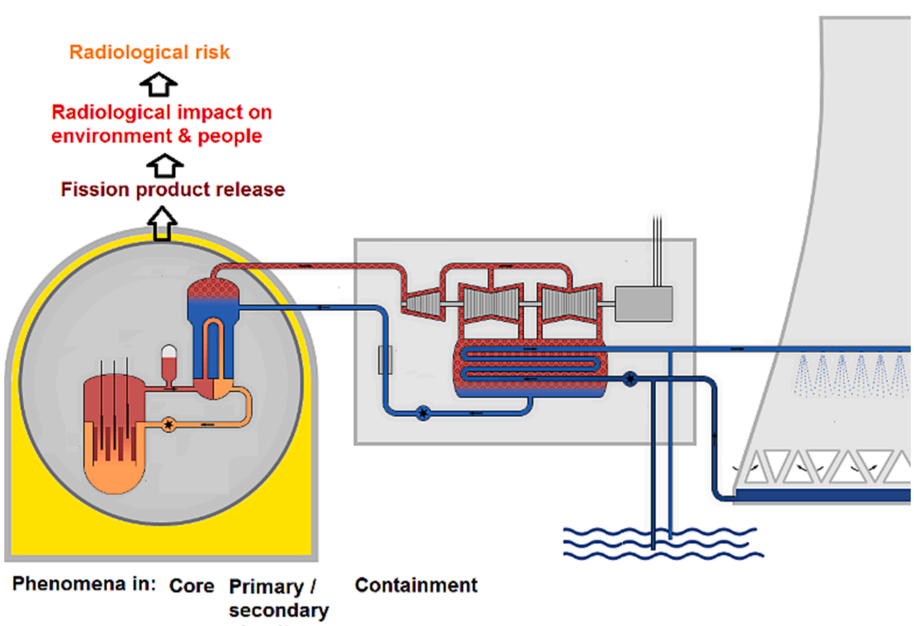


Fig. 1. Scheme of a Pressurized Water Reactor with key-components (Core, primary/secondary, and containment) and the path for the release of fission products determining the radiological risk.

input to the output of any neutronic, TH, etc. The acceptance of numerical tools for safety assessment by the end users depends on the degree of validation, where the availability of experimental data for specific phenomena and reactor design is fundamental. KIT has operated a large number of experimental facilities relevant for the validation of design basis and severe accident codes e.g. the COSMOS and QUENCH facilities built for LWR e.g. PWR, VVER, but also with potential use for water-cooled SMRs and PWR Gen III reactors.

The paper starts with the description of the overall KIT strategic approach for the development of sophisticated numerical simulation routes for both design basis and severe accidents based on in-house and external codes in Chapter 2. The numerical tools for the analysis of design basis accidents are briefly described in Chapter 3, whereas severe accident tools under use and validation are described in Chapter 4. The KIT code for the prediction of the radiological dispersion after hypothetical core meltdown accidents is presented in Chapter 5 while the new KIT Python-based tool for the quantification of uncertainties and sensitivities of different e.g. TH, neutronics tools is discussed in Chapter 6. In Chapter 7, the multi-physics coupling approaches under development for improved core analysis combining in-house TH codes with external neutronic and thermo-mechanics solvers are presented, and selected applications are discussed. The multi-scale/-physics coupling approaches for improved plant analysis that combines system TH codes with subchannel and CFD-codes are presented in Chapter 8. Selected KIT experimental facilities for investigations of safety-relevant TH and severe accident phenomena for LWR, SMR, and Accident Tolerant Fuel (ATF) are presented in Chapter 9 including selected validation work. A summary and outlook are provided in Chapter 10.

2. KIT strategy for the prediction of the overall risk from severe accidents

The KIT strategy for the development of required numerical tools for the estimation of the radiological risk that may arise from hypothetical severe accidents with considerable release of radioactive material into the environment is based on the following pillars:

- In-house tools for core physics including depletion (to predict nuclide inventories),
- International tools for the simulation of integral NPP-behavior under severe accident conditions with a massive release of radionuclides, and
- In-house tools for the estimation of the radiological impact on the NPP-site i.e. on the environment and people.

In Fig. 2, the numerical tools under use, development, and validation at KIT for the core, the plant, and the radionuclide dispersion are shown.

In Fig. 3, the list of in-house and external numerical tools for the core and plant analysis under design basis accidents is shown. The codes written in black are KIT-developments while the others are international tools being used at KIT in the frame of long-term international co-operations e.g. the US NRC CAMP-agreement that offer full access to the source codes of e.g. PARCS, TRACE, RELAP5. Other codes such as the Monte Carlo code SERPENT2 (SSS2) and TRANSURANUS (TU) are used based on bilateral co-operations with VTT and JRC Karlsruhe.

Apart from using the well-established system TH codes coupled with 3D nodal diffusion core analysis tools, KIT started the development of multi-physics/-scale methods by combining sophisticated TH solvers (CFD, subchannel, porous-media) with neutronic deterministic (sp3, spherical harmonics) and stochastic (Monte Carlo) for very detailed core analysis at pin/subchannel (PWR, VVER, SMR) or plate/subchannel (Material Testing Reactors: MTR) level simulations. Such developments are worldwide driven by advances in computation methods, the increasing computational power of High-Performance-Computation (HPC) clusters, and last but not least the continuous improvement of safety analysis tools dealing with the core and plant behavior. In addition, the validation of the neutronic and TH codes for reactor safety is primordial. Hence, KIT uses experimental data obtained in both in-house and external test facilities including separate, coupled, and integral tests as well as plant data.

Regarding the strategy for the development of in-house numerical tools and the validation of own and external tools used at KIT for safety-related investigaitons, it can be stated that the KIT-strategy relies on the combination of numerical simulations (inhouse and external codes) and experimental investigations (in-house and external tests). In Fig. 4, the strategy for code development and validation for both design basis and beyond design basis accidents followed at KIT is shown. There, both inhouse code developments and test facilities are highlighted in red. All listed tools except ASTEC and MELCOR are thermal hydraulic tools of different details and modeling scope used mainly in the field of design basis accidents. On the left side, selected experimental facilities used at KIT for code validation in the respective areas are listed.

3. Numerical tools for the analysis of design basis accidents of LWRs

Most system TH tools contain 1D TH models for a large number of flow regimes and heat transfer models covering the whole boiling regime. In the last decades, 3D coarse mesh TH models were added to RELAP5-3D (INL, 2018), TRACE (USNRC, 2013), CATHARE-3D (Bestion, 1990), and ATHLET (Lerchl et al., 2019) to improve the simulation of 3D phenomena taking place within the core, the RPV, the primary and secondary circuits. In the meantime, the analysis of the core behavior of LWR using coupled codes based on 3D nodal diffusion solvers and 3D coarse mesh TH system codes such as TRACE/PARCS can be done with detailed core models, where each fuel assembly is represented by one neutronic node and one TH mesh, i.e. a 1-to-1 mapping of the neutronic and TH domain. This approach makes the grouping of fuel assemblies (FA) of a core with e.g. 193 FAs into 30 groups meaning 30 TH channels mapped to 193 neutronic nodes unnecessary. Such kinds of simulations are feasible thanks to the huge and cheap computer power fast enough for industry-like applications with sufficient accuracy.

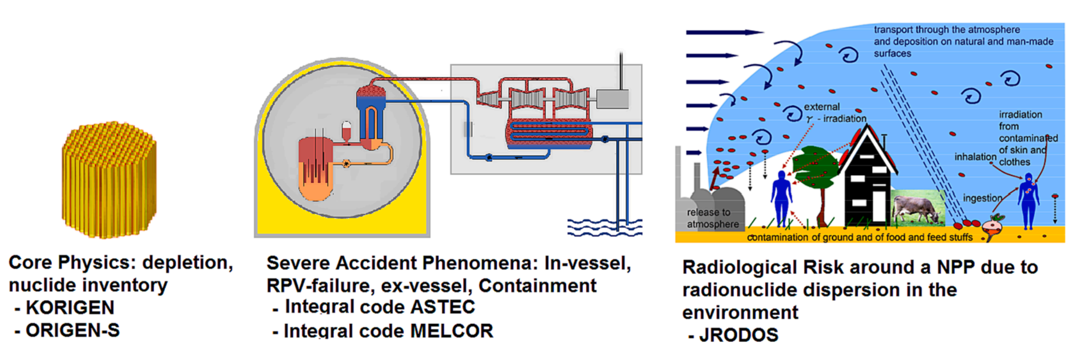


Fig. 2. Overview of numerical tools for the prediction of the radiological dispersion after a hypothetical severe accident.

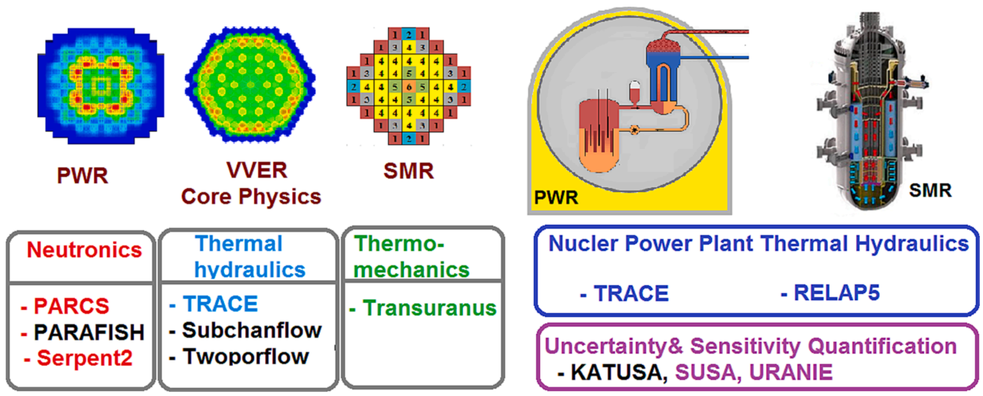


Fig. 3. KIT computational route for the safety assessment of design basis accidents of different nuclear power plant designs (tools in black are in-house developments, the rest are external tools).

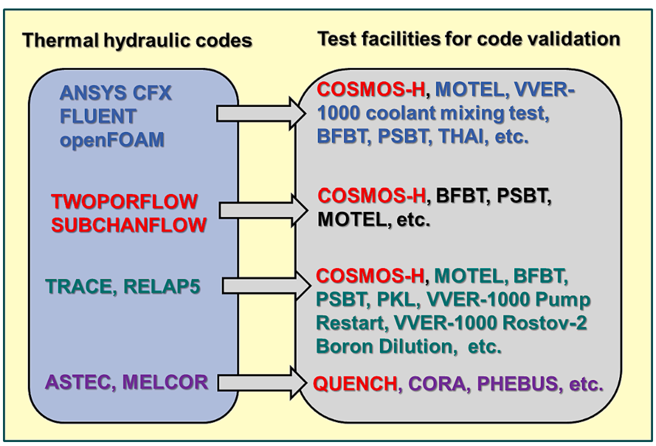


Fig. 4. Scheme of the KIT strategy for the development and validation of thermal hydraulic codes.

At present, the core THs of e.g. a PWR can be represented by a 3D Cartesian VESSEL-component of TRACE, where one fuel assembly is represented by one radial mesh. In this approach, the mass, momentum, and energy conservation in the R-, Z-, and –azimuthal direction is considered simply. On the other hand, large efforts were undertaken worldwide and also at KIT to extend the capability of subchannel codes such as CTF (Salko and Avramova, 2015), Subchanflow (Imke and Sanchez, Validation of the Subchannel Code SUBCHANFLOW Using the NUPEC PWR Tests (PSBT), 2012), FLICA-IV (Toumi et al., 2000), etc. to perform fuel assembly or subchannel level simulations of LWR-cores with square or hexagonal geometry. In parallel, 3D TH codes based on the porous media and a two-phase flow approach with improved physics were developed such as PORFLO (Ilvonen et al., 2010), CUPID (Jeong et al., 2010), TWOPORFLOW(TPF) (Trost et al., 2013) to overcome the limitations of the 3D coarse mesh system TH modules.

The ultimate goal of numerical tools for safety evaluation is the capability to predict local safety parameters (maximal fuel/cladding temperature, Departure of Nucleate Boiling Ratio (DNBR)) in a direct manner avoiding the use of hot channel factors. This goal can be achieved by coupling neutronic solvers (Monte Carlo or deterministic transport codes) with subchannel codes and applying such coupled codes to simulate the behavior of LWR-cores under accidental conditions (Gomez et al., 2012; Daeubler et al., 2015; Ferraro et al., 2021; Garcia, 2021).

The KIT research activities on reactor safety focus on gradually increasing the prediction accuracy of numerical tools for reactor safety evaluations by developing subchannel and porous-media 3D TH codes as well as deterministic transport codes together with the use of Monte Carlo solvers. These developments are complemented by the development of multi-physics and multi-scale coupling methods and increasingly considering advanced deterministic/stochastic neutronic and thermo-mechanic solvers. In subsequent chapters, more details about these developments will be described, and selected results will be presented.

3.1. KIT thermal hydraulic core analysis tools

The focus of KIT is on the development of improved TH tools for the core analysis compared to the system TH codes. Consequently, sub-channel and porous-media codes with 3D models are being developed to fill the gap between CFD (very CPU intensive) and system codes (mainly 1D and simplified 3D physics) for different core designs including the one of BWR, PWR, VVER, and research reactors with MTR-fuel. The sub-channel code SUBCHANFLOW (SCF) and the porous-media two-phase flow code TPF have been developed and validated at KIT for many years.

SCF is a fast-running and flexible sub-channel code that can handle rectangular, hexagonal, and plate fuel bundles as well as whole core geometries. It is based on the legacy COBRA-code family, (Rowe, 1973; Wheeler et al., 1976), and (Basile et al., 2010). Modeling is concentrated on the main physical phenomena occurring in sub-channel flow for steady state and transient conditions in consideration of fast and stable execution. In a basic option steady state and transient problems are solved with an iteration-based COBRA-like fully implicit solver, so the flow is restricted to an upward direction with the lateral exchange. In addition, a solver is available which allows low flow rates, downward flow, and buoyancy-driven flow. It is based on the semi-implicit SOLA method (Hirt et al., 1975). Coolant properties and state functions are implemented for water using the IAPWS-97 formulation. In addition, property functions for liquid metals (sodium and lead) and gases (helium, air) are available. Two-phase flow (boiling) is implemented for water and sodium. The heat transport from the nuclear-heated fuel rods to the fluid is based on a cylindrical 1D radial heat conduction model including the gap conductance between the fuel pellets and the cladding. As boundary conditions, the total flow rate or a channel-dependent flow rate can be selected. It is possible to distribute the flow automatically to the parallel channels depending on the friction at the bundle inlet. In addition, a pure top–bottom pressure difference boundary can be used. Fluid temperature at the inlet and pressure at the outlet always have to be prescribed as boundary conditions. An iterative steady-state numerical procedure is available to determine the power at which critical heat flux conditions appear during the simulation. In SUBCHANFLOW, profit is taken from the many valuable empirical correlations for pressure drop, heat transfer coefficients, and void generation collected over the last decades. Consequently, it does not follow the general trend to describe two-phase flow by simulating the processes on a microscale basis, e.g. separate conservation equations for liquid droplets, films, or vapor bubbles. In SUBCHANFLOW, a three-equation two-phase flow model that is a mixture equation for mass, momentum, and energy balance is implemented. The constitutive relations are expressed as mixture equations for wall friction and wall heat flux as well as a two-phase flow slip velocity correlation. Boron transport can be tracked in a manner that conserves strong concentration gradients. The main calculation routines are allowed to be controlled by a series of C programming language function interfaces. They permit to use of SCF as an external precompiled library, to exchange all the data necessary for coupled neutron physics calculations. The input is oriented to a text-based user interface using comprehensive keywords and simple tables.

Validation work is performed using relevant data for PWR, BWR (Imke and Sanchez, Validation of the Subchannel Code SUBCHANFLOW Using the NUPEC PWR Tests (PSBT), 2012), (Sánchez et al., SUBCHANFLOW: A Thermal-Hydraulic Sub-Channel Program to Analyse Fuel Rod Bundles and Reactor Cores, 2010). SCF is coupled with different neutronic solvers based on diffusion (PARCS), simplified transport (DYN3D-SP3), and Monte Carlo (MCNP5, SERPENT2) for static and dynamic coupled simulations of core transients. In Fig. 5, different fuel assemblies and core arrangements are shown which can be analyzed with SCF stand-alone or coupled with different neutronic solvers (deterministic and Monte Carlo).

TPF is a 3D TH transient computer code that solves the two-fluid equations describing two-phase flow including boiling and heat-transfer dynamics related to a heated solid structure. The development started in 2000 to calculate single- and two-phase flow heat transfer in microchannel heat exchangers (Imke, 2004; Trost et al., 2013). Currently, TPF is mainly used to simulate the TH inside a nuclear reactor core (Jauregui-Chavez et al., 2018). Here 3D phenomena may be important but the application of CFD tools using body-fitted meshes to resolve the complex geometry is still computationally very expensive. As the code name implies, the porous medium approximation is employed in the whole simulated domain to model the geometrical details not explicitly represented in the mesh to reduce the computational requirements. The exact local flow field within the given geometry is not calculated, but the physical phenomena are averaged over a selected volume that contains both fluid and solid phases.

The two-fluid model uses separate partial differential equations expressing the conservation of mass, momentum, and energy for each fluid phase. Empirical expressions for the exchange of mass, momentum, and energy between the phases are necessary to close the system. In addition, the friction and the heat transfer related to the solid structure have to be modeled. The representation of flow is based on a Cartesian mesh well suited for assembly-wise core analysis or the simulation of single rod bundles similar to the application of sub-channel codes, but using the full set of equations.

To solve the fluid dynamic equations, a semi-implicit technique is used in connection with a staggered mesh locating momentum at the cell boundaries and locating all scalar quantities at cell centers. The mass and energy equations written in finite volume form are combined with the finite difference momentum equations to yield a single system of equations for pressure. From the resulting pressure field, the velocities are obtained directly. The equations are linearized in their implicit parts and only the first step of a Newton-Raphson iteration is taken at each time step. Convergence to a steady state can always be reached if the time step size is sufficiently small. Apart from the porous media approach, the heat transport from the nuclear-heated fuel rods to the fluid is based on a cylindrical 1D radial heat conduction model including the gap conductance between the fuel pellets and the cladding. For several rods aggregated in one computational cell, a representative average fuel rod is used. A continuous general boiling curve describing the heat transfer from the cladding surface to the fluid below and above critical heat flux (CHF) is derived from empirically modeled basic flow regimes. TPF combines a two-phase flow model with a well-known reliable numerical method. However, a careful selection and assessment of the constitutive equations are needed for accurate predictions. Different correlations of heat transfer in the pre-CHF up to CHF conditions such as the Biasi, Bowring, Westinghouse-3, and Groeneveld Look-up table were implemented and validated recently (Jauregui-Chavez et al., 2018) and (Jauregui-Chavez V. , 2020).

3.2. *KIT neutronic core analysis tools*

3.2.1. *Depletion solver KORIGEN*

The depletion analysis of different reactor cores is performed at KIT with the in-house code KORIGEN (Wiese, 1998). In addition, international tools such as the ORIGEN-S of the Scale system, (Wieselquist, 2015), the commercial CASMO5 (Hykes and Ferrer, 2013), or Serpent2 (Leppänen et al., 2013) can be also used. These codes allow the prediction of fuel isotopic depletion, decay heat, activation, and source term for any kind of core loadings.

3.2.2. *Transport solver PARAFISH*

KIT is developing the PARAFISH code based on a deterministic neutron transport solver with even parity formulation (Criekingen et al.,

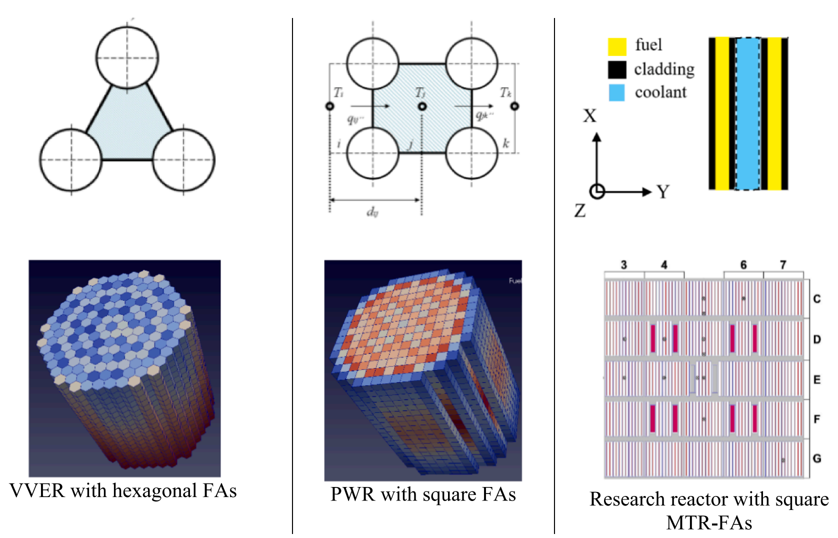


Fig. 5. Arrangements of different hexagonal and square power reactor cores and research reactor cores (bottom) with different coolant channels (top). triangular, square, and narrow rectangular.

2011). It can perform calculations on 2D/3D Cartesian geometries in steady-state for a multiplying media. The methodology discretization follows the multi-group approximation for the energy variable, non-conforming finite elements for the spatial variables, and spherical harmonics expansion (P_N) for the angular variable. Currently, the code is written in Fortran 90. It employs the numerical library PETSc for solving the linear systems built by discretization (inner iterations). Regarding the k_{eff} calculation, the classical Power Method (outer iterations) is used, since it offers a simple procedure. PARAFISH has been verified with some classical benchmarks (Duran-Gonzalez et al., 2022; Duran-Gonzalez et al., 2022), obtaining encouraging results. Recently, more challenging problems e.g. a heterogeneous reactor without spatial homogenization such as the Benchmark C5G7 (Lewis et al., 2003) are being simulated to demonstrate the prediction capability, see Fig. 6. Ongoing enhancements focus on NEMTAB format reading implementation, anisotropic scattering, and employing the SLEPc library.

The focus is now on the extension of the time-dependent capability for the analysis of transient SMR cores in the frame of the national BMBF project InnoPool-SMR-safety. SMR-cores are characterized by a harder spectrum, high leakage of neutrons due to their compactness requiring a multi-group approach with more than two energy groups and the use of transport solver to properly describe the high heterogeneity in the radial and axial direction, where the diffusion approximation maybe not sufficient. It will be coupled with TH core analysis codes such as SCF and TPF. The validation process is ongoing in the frame of international OECD/NEA activities (Duran-Gonzalez et al., 2022).

3.3. System thermal hydraulic codes for the analysis of design basis accidents

In the frame of the international code assessment and maintenance program (CAMP) of the US NRC, KIT obtained access to the source code of the system TH codes RELAP5 (NRC, 2010) and TRACE (USNRC, 2013) as well as the core simulator PARCS (Downar et al., 2012) since many decades. TRACE is the new reference computer code of the US NRC for LWR and innovative reactors. It is extensively validated by a large international community in the frame of CAMP. KIT was involved in the validation of TRACE for its application to PWR (Jaeger and Sánchez Espinoza, 2013; Sánchez et al., 2007), VVER (Sánchez-Espinoza and Böttcher, 2006; Redondo-Valero et al., 2023), BWR (Jaeger et al., 2013; Hartmann C. , 2016), and SMR (Sanchez-Espinoza et al., 2018) reactors using experimental and plant data of VVER, BWR (Hartmann et al., 2011), and GEN-IV (Jaeger et al., Thermal-Hydraulic Evaluation of an LBE Cooled 19 Pin Bundle in the Frame of TRACE Validation, 2013) reactors for many decades as part of international benchmarks and national activities.

In addition to the validation of the TH models of system codes, the OECD/NEA activities of the last decades were concentrated on the validation of the simulation capability of coupled 3D neutron diffusion solvers with system TH codes e.g. RELAP5/PARCS, TRACE/PARCS, ATHLET/CUBOX-QUABOX, ATHLET/KIKO3D, CATHARE/CRONOS2, RELAP3D/NESTLE, etc. in the frame of different benchmarks such as the TMI-1 MSLB (Ivanov et al., 1999), BWR Turbine Trip-2 (Solis et al., 2001), V1000 Coolant Transient 1 (Ivanov et al., 2002), V1000 Coolant Transient 2 MSLB (Kolev et al., 2006), Kalinin-3 Coolant transient (Tereshonok et al., 2008), and the Boron Dilution Rostov2 (Avramova et al., 2020), where real plant data was provided to the participants for code validation. KIT participated in selected benchmarks using the US NRC coupled codes RELAP5/PARCS (Sánchez-Espinoza and Böttcher, 2006) and TRACE/PARCS (Jäger et al., 2008). In recent years, KIT's focus was on the development of multiscale TH coupled methods combining system TH codes with sub-channel and CFD codes to improve the simulation of 3D phenomena inside the core and within the reactor pressure vessel for large PWR, water-cooled SMR with integrated RPV and research reactors loaded with MTR-fuel plates. For the coupling of TRACE with the in-house code SCF both the external communication interface (ECI) (Zhang and Sanchez-Espinoza, 2020) of TRACE as well as the ICoCo-approach (Zhang et al., 2021) were implemented. More details of this development can be found in a recent publication (Sanchez-Espinoza et al., 2023).

4. Numerical tools for the analysis of beyond design basis accidents

The Fukushima accident underlined the importance of fast-running severe accident codes with the best physical models and mathematical formulation to be used to extend the technical basis for the optimization and development of appropriate Severe Accident Management measures (SAM) for LWR (Sanchez et al., 2015) and (Dorsselaere et al., 2015). In (Sanchez et al., 2016), the KIT investigations for designs and beyond design basis accidents are described. For the analysis of hypothetical severe accidents in nuclear power plants, KIT builds on two strategic cooperations:

- Cooperation with IRSN that permits KIT full access to the source code of the European severe accident code ASTEC (Accident Source Term Evaluation Code). This integral code is being developed by IRSN to simulate the entire severe accident sequence from the initiating state to the release of radioactive material to the environment (Chatelard et al., 2016; Chatelard et al., 2016). In the frame of the NUGENIA ASCOM project, different institutions of the EU and the world are using the ASTEC for validation and application to analyze severe accidents in different reactor designs and spent fuel pools. Besides, ASTEC is being applied and validated in the frame of different European projects such as SARNET (Albiol et al., 2010), CESAM (Nowak et al., 2018), MUSA (Herranz et al., 2021), etc. The goal is to extend the validation matrix and application to reactor designs under operation in Europe and to the ones under planning. KIT is actively participating in these international activities as a premium partner of IRSN with full access to the source code. Results of the validation and verification of the different models are published in (Fichot et al., 2017; Belon et al., 2017; Chatelard et al., 2017). In recent EU projects e.g. SASPAM-SA, ASTEC is being applied to water-cooled SMR. In ASSASS, the potential use of artificial intelligence is being evaluated and explored for implementation in ASTEC to speed up severe accident simulations. Finally, it is worth mentioning that the application and adaptation of ASTEC for the analysis of accidental scenarios in fusion facilities and spent fuel pools is another important topic of investigation.
- Participation of KIT in the international cooperative severe accident research program (CSARP) of the US NRC for many years has paved the way for KIT to use the reference severe accident code MELCOR (Humphries et al., 2015; Humphries et al., 2015) of the US NRC for validation and application to different reactor designs. The CSARP's objective is the exchange of experimental data and analytical research in severe accidents. In the frame of CSARP, KIT obtained access to the USNRC reference severe accident code MELCOR. It is an integrated, engineering-level computer code whose primary purpose is to model the progression of postulated severe accidents in light-water reactors and in spent fuel pools.

At KIT, key experimental facilities e.g. QUENCH, LIVE, HYKA, DISCO, and MOCKA devoted to investigating severe accident phenomena provide important data for code validation (Steinbrück et al., 2010; Miassoedov et al., 2013; Miassoedov et al., 2012), and (Miassoedov et al., 2013) for many years. The validation work contributes to a better understanding of the core melt sequences and thus improves the safety of existing and, in the long-term, Gen-III and –IV reactors by severe accident mitigation measures. KIT experiments are part of the SAFEST (Miassoedov et al., 2015) and ALISA (Zhang et al., 2012) projects of the 7th EU Framework Programs. The analytical work is focused on the improvement and validation of severe accident codes such as ATHLET-

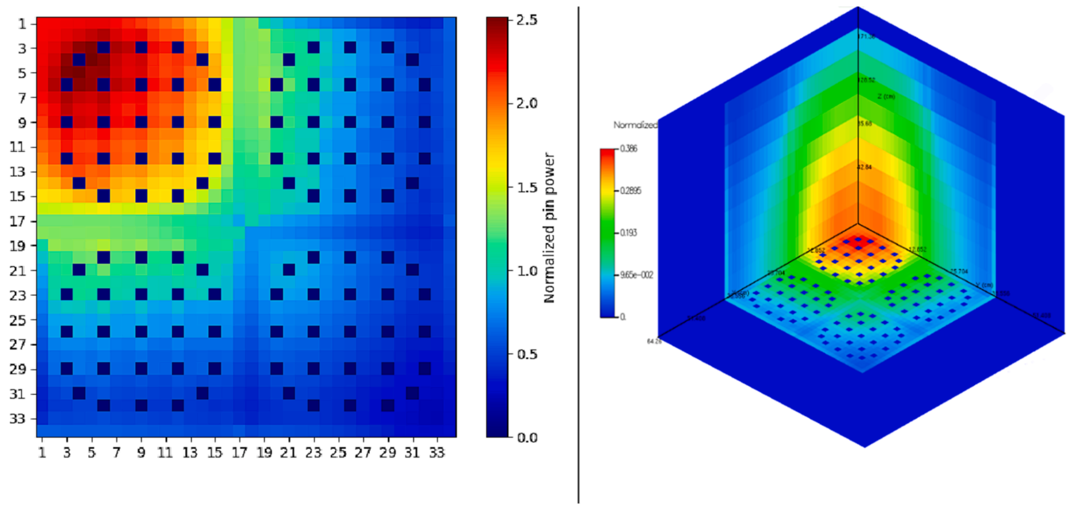


Fig. 6. Analysis of the C5G7-3D benchmark with PARAFISH; (left). Overall Pin Power Distribution, (right). 3D Power Density Distribution.

CD, ASTEC, and MELCOR in the frame of international and national projects (WASA-BOSS, CESAM) e.g. lower head models, coupling of integral codes e.g. MELCOR with CFD-like code (GASFLOW) for an improved description of containment phenomena (Szabó, 2014). Validated severe accident codes, (García-Toraño et al., ASTEC Validation based on the KIT Re-flooding Experiment QUENCH-08, May 6–8 2014) and (DiMarcello et al., 2014, May 6–8), are then used for the simulation of severe accident sequences of PWR (García-Toraño et al., 2015) and (García-Toraño et al., Investigation of SAM measures during selected MBLOCA sequences along with Station Blackout in a generic Konvoi PWR using ASTECV2.0, 2017) and BWR aiming to improve the SAM guidelines based on the insight gained from the simulations (García-Toraño et al., 2015) and (DiMarcello et al., 2015).

Recent investigations are focused on the validation and application of ASTEC to analyze the progression of different severe accident sequences in generic VVER-1000 (Mercan et al., 2022), GE BWR (Murat et al., 2023), and KONVOI. Other than the analysis of the in- and ex-vessel progression of selected severe accident sequences, such activities aim at performing the prediction and the uncertainty quantification of the source term. Such analyses are carried out by propagating the uncertainty of selected ASTEC input variables on the amount of the fission products released by the core during the accident and transported to the containment and then the environment, as more extensively discussed in the following chapters.

All the calculation options are activated in the ASTEC model to fully consider the main in-vessel and ex-vessel phenomena occurring during the analyzed severe accident scenarios. Namely, the main physical models governing the chemical interactions, the heat exchange, and the magma creation and movement are considered. Furthermore, particular attention is devoted to the models governing the fission product release and transport. The ASTEC model of the generic VVER-1000 NPP developed at KIT and the analyses of the results of a severe accident sequence initiated by a Large Break Loss of Coolant Accidents (LBLOCA) (850 mm break in the cold leg) in conjunction with a Station Black Out

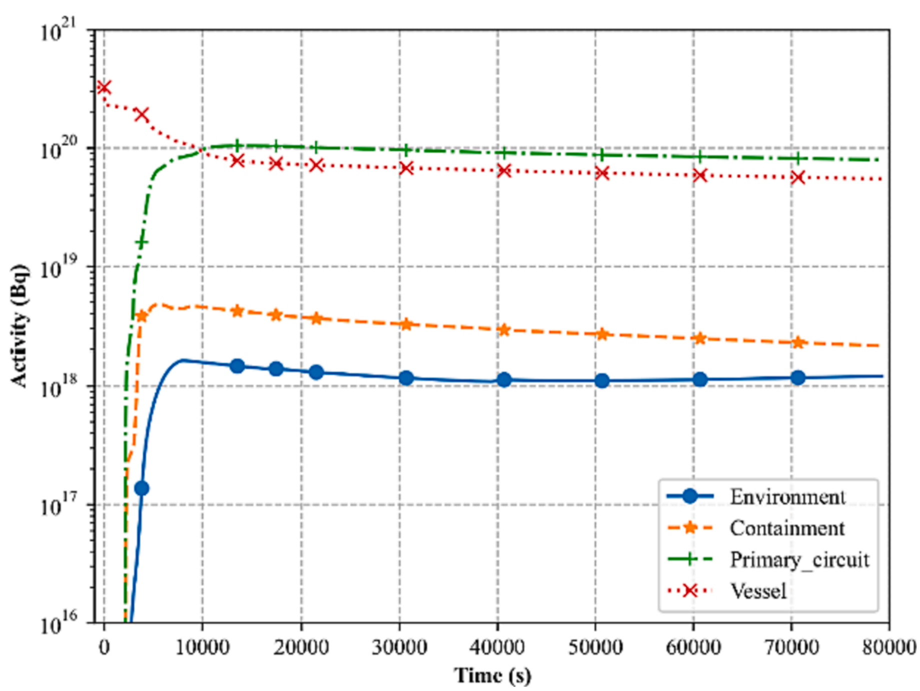


Fig. 7. Total activity in the plant and in the environment during an LBLOCA + SBO scenario in a generic VVER-1000 (Mercan et al., 2022).

(SBO) are described in (Mercan et al., 2022). The fuel inventory loaded in the core is evaluated using the KORIGEN tool and the scenario is simulated from the initiation up to the basemate rupture. The total activity in the vessel, in the primary circuit, in the containment, and the environment during the scenario are shown in Fig. 7. Despite the large retention in the primary circuit (about 99% of the initial fuel loading), the total activity in the containment ranges between 2E18 Bq and 3E18 Bq, and the amount released reaches about 1.20E18 Bq. To perform a deep investigation of the source term, the ASTEC code also allows calculating the element- and isotope-wise mass of all fission products transported from the core to the environment as well as the corresponding activity. Having this in mind, the activity of the relevant isotopes mostly affecting the source term at the end of the scenario (about 80,000 s) is shown in Fig. 8. The results show that high-volatile isotopes (Xe^{133} and Xe^{135}) mainly affect the source term.

The ASTEC model of the generic Peach Bottom Unit-2 BWR4 Mark-1 reactor developed at KIT and the analyses of the results of the ST-SBO scenario are described in (Murat et al., 2023). It is worth noting that such a model is the first application of the ASTEC code to BWR technologies outside IRSN. Furthermore, the model employs the most recent ASTEC developments related to BWRs, i.e. fuel channel boxes. The fuel inventory loaded in the core has been computed by employing the SCALE V6.2b code system, the ORIGEN module being employed for fuel depletion calculations. ASTEC model of the containment and the reactor building is shown in Fig. 9. The amount of Xe, I, and Cs in the containment and released to the environment during the scenario is shown in Fig. 10 and Fig. 11 respectively, as a fraction of the initial loading in the core. The results show that the fraction of the initial loading of Xe and I released to the environment is about 10% and 3%, respectively (Murat et al., 2023). The ASTEC results are in good agreement with previous MELCOR studies.

The ASTEC model developed at KIT for the containment of the generic KONVOI plan is shown in Fig. 12. The containment is modeled through 26 rooms plus an auxiliary building. In Fig. 12, the plant (green, red, gray, and light blue boxes), the operating (white boxes), and the annulus (light yellow boxes) rooms are shown. The containment and the annulus are connected with the environment through fans (light blue arrows). Given a reliable evaluation of the source term, efforts have been spent to properly evaluate the fuel inventory at the equilibrium. With this goal, the core has been loaded with 193 FA composed of 48 U FA (6 batches), 81 U-Gd FA (6 batches), and 64 MOX FA (4 batches). The ORIGEN ARP tool has been employed to evaluate a library of fuel inventories in each 30 effective full power days (efpd) for a total of 328 efpd. As discussed in (Murat et al., 2023) an ASTEC database of different severe accident scenarios has been assessed. As an example, the time-dependent evolution of the amount of Xe, I, and Cs aerosols, as a fraction of the initial loading, in the containment during a Medium Break Loss of Coolant Accident (MBLOCA) (12′′ break on the cold leg) scenario is shown in Fig. 13. In particular, the results obtained by employing the fuel inventories computed at the middle and at the end of the cycle, MBLOCA and End of Cycle (EOC) respectively, are shown. As expected, almost all the Xe inventory is transported from the core to the containment in both scenarios. The fraction of Cs aerosols reaches about 10% of the initial inventory at about 20,000 s, corresponding to the rupture of the vessel. Furthermore, it can be observed that the amount of I aerosols in the containment strongly depends on the fuel inventory loaded in the core. The results in Fig. 13 reveal a higher amount of I aerosols (up to 10% of the initial inventory) when a fuel inventory with higher burn-up is employed.

5. KIT tool JRODOS for the prediction of radiological dispersion into the environment after severe accidents

An important objective of the KIT activities is the estimation of the radiological impact after hypothetical severe accidents with core meltdown for reactor designs that are under operation in Europe using the JRODOS code. As mentioned in Chapter 2, Fig. 2, a whole chain of computational tools among other severe accident codes such as ASTEC, and MELCOR are needed to predict the radiological source term that potentially may be released in hypothetical severe accident sequences. This information is needed by tools like JRODOS for the estimation of the radiological consequences for the environment and population around the NPP. In 1986, after the Chernobyl accident, KIT started the development of the RODOS (Real-time On-line Decision Support) system within several European research programs to support decision-making in case of a nuclear or radiological emergency (Ehrhardt and Weis, 2000). In the frame of the EURANOS project, the code was redesigned based on user requirements and updated to the JAVA environment (now named JRODOS) (Levdin et al., 2010), Fig. 14. JRODOS can be used in national or regional emergency centers, providing coherent support at all stages of an accident (i.e., before, during, and after a release), including the long-term management and restoration of contaminated areas. The system can support decisions about the introduction of a wide range of potentially useful countermeasures such as sheltering and evacuation of people, distribution of iodine tablets, food restrictions, agricultural countermeasures, relocation, decontamination, or

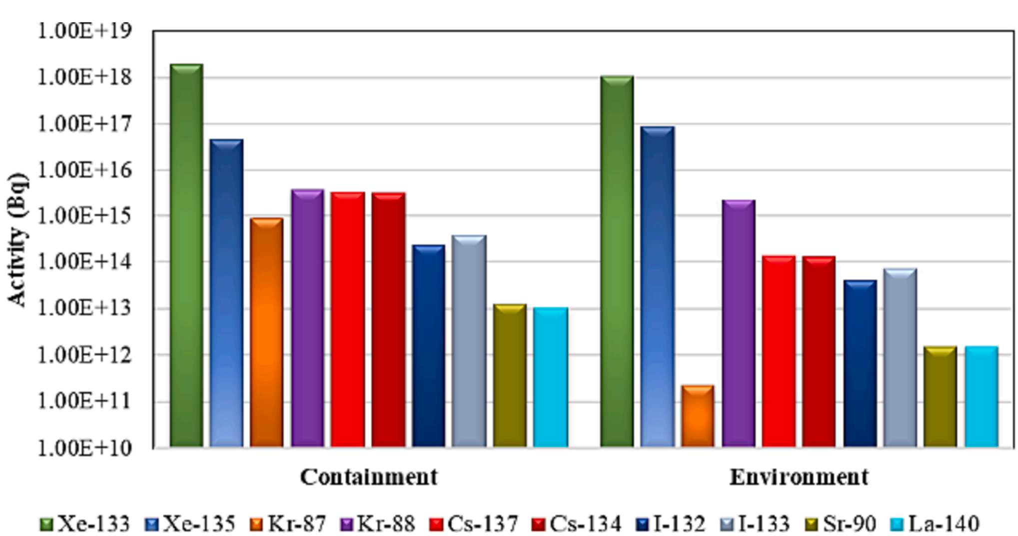


Fig. 8. Isotope-wise activity in the containment and in the environment at the end of the ASTEC calculation of a LBLOCA + SBO scenario in a generic VVER-1000 (Mercan et al., 2022).

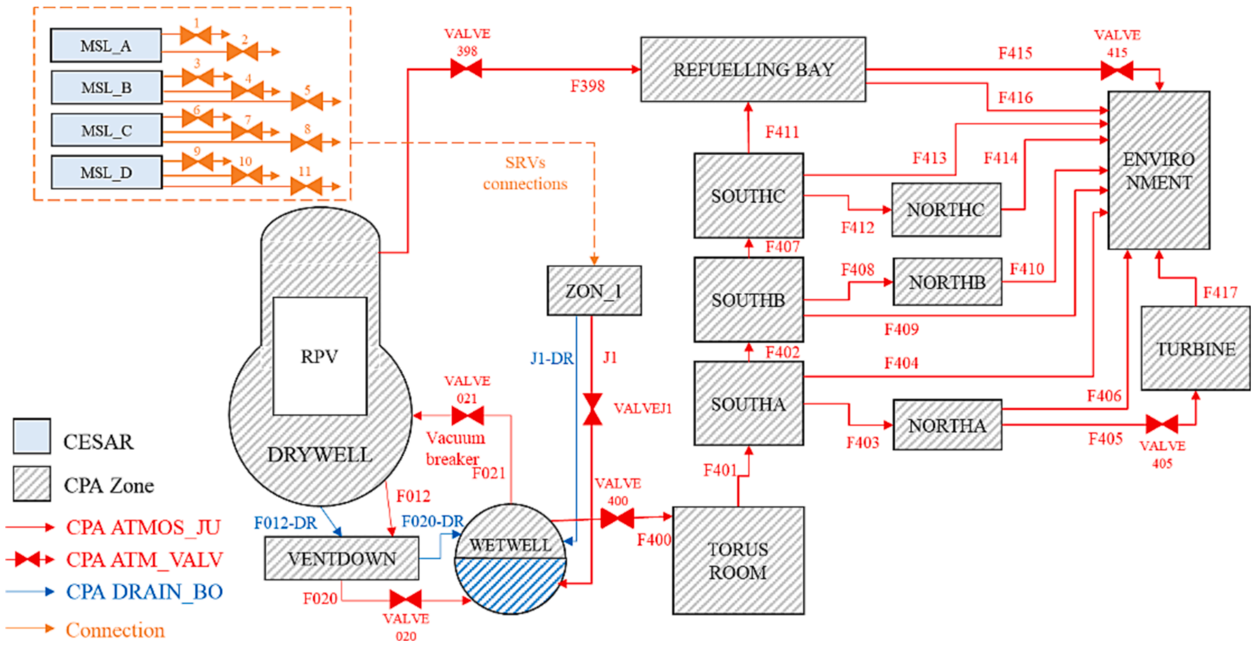


Fig. 9. Primary containment, vessel, and reactor building sections of the ASTEC model of a generic Peach Bottom Unit-2 Reactor (Murat et al., 2023).

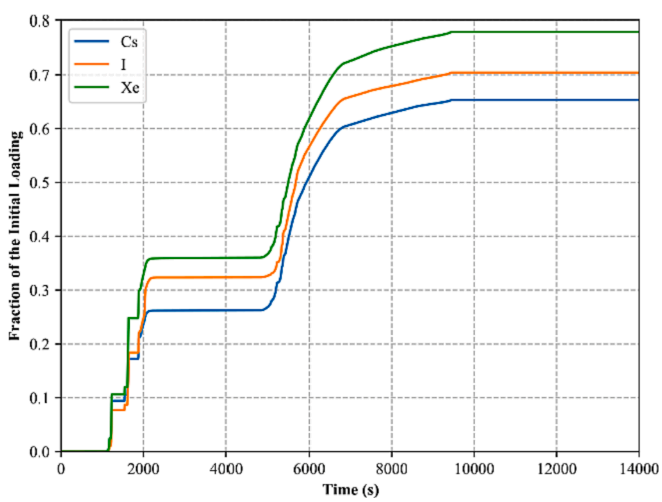


Fig. 10. Evolution of the Xe, I, and Cs in the containment during an ST-SBO in the ASTEC model of a generic Peach Bottom Unit-2 Reactor (Murat et al., 2023).

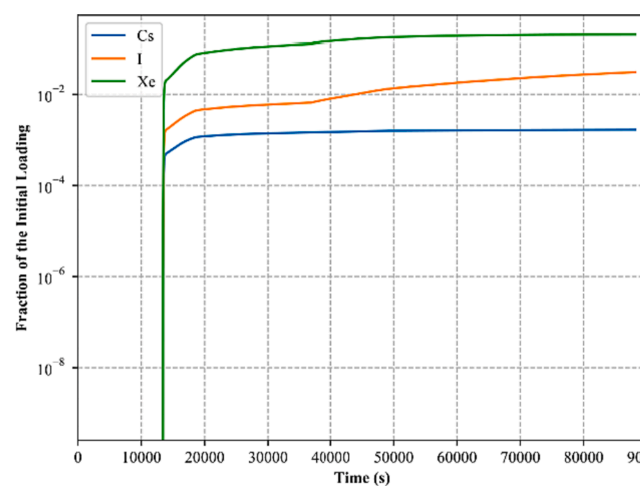


Fig. 11. Evolution of the Xe, I, and Cs released to the environment during an ST-SBO in the ASTEC model of a generic Peach Bottom Unit-2 Reactor (Murat et al., 2023).

restoration, mitigating the consequences of an accident concerning health, the environment, and the economy. It can be applied to accidental releases into the atmosphere and various aquatic environments. Appropriate interfaces exist with local and national radiological monitoring data, meteorological measurements and forecasts, and for adaptation to local, regional, and national conditions worldwide. The most important JRODOS module to be used in the early phase of an emergency is the Emergency Model Chain (EMC). The chain contains several simulation models such as atmospheric transport and dispersion, behavior of the radionuclides in the food chain, and countermeasure simulations.

To facilitate atmospheric transport and dispersion calculations for different purposes, three simulation models are implemented in JRODOS:

- RIMPUFF, (Mikkelsen et al., 1984), for fast assessments in the very early phase (puff model for simple conditions)
- DIPCOT (Andronopoulos et al., 2010; Davakis et al., 2003; Janicke, 1994) and
- LASAT for assessments under complex meteorological conditions.

JRODOS is now applicable to the whole world containing databases on topography, land use, and soil type necessary to run the simulation models. All commercial nuclear power plants are part of the system too. An important aspect is the information needed for the system in case of an emergency such as meteorological weather data and source term. Numerical weather data can be provided by the National Weather Service – typically for a forecast over 48 h – or from the US NOMADS server.[1] With the many end users, JRODOS has reached operational maturity and is a key component for nuclear and radiological emergency management in more than 40 countries worldwide, once the ongoing

[1] Data from the Global Forecast Systems (GFS), cf. https://nomads.ncep.noaa.gov/.

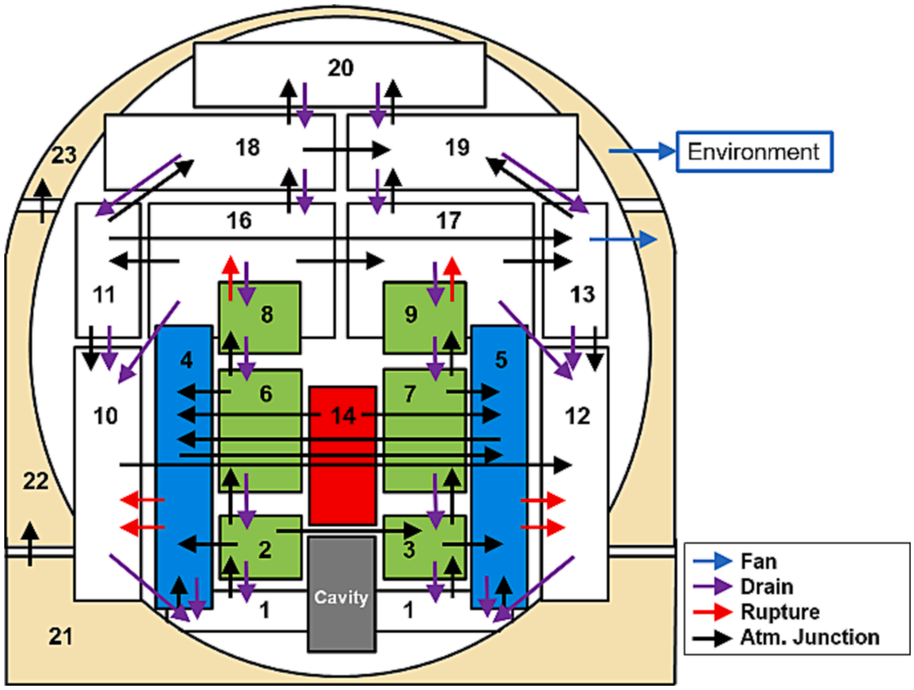


Fig. 12. ASTEC containment model of a generic KONVOI NPP.

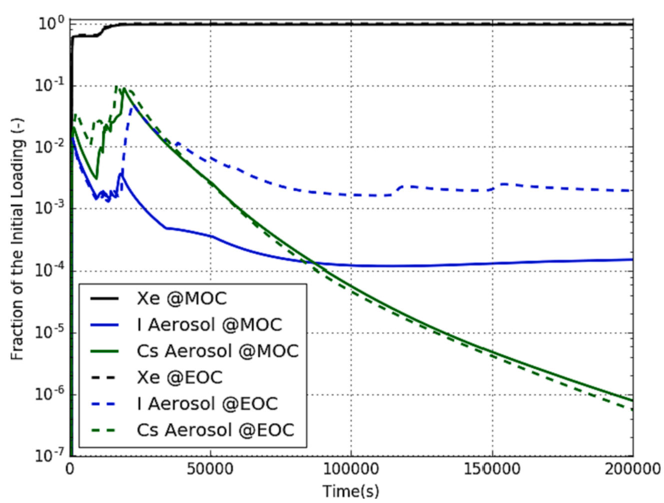


Fig. 13. Amount of Xe, I, and Cs aerosols in the containment as a fraction of the initial fuel mass in the core in the MBLOCA scenarios.

installations are completed, Fig. 15.

For many years, the computational route shown in Fig. 2, has been extensively used to predict the radiological risk of hypothetical severe accidents in NPPs of type VVER-1000 (Mercan et al., 2022), GE BWR (Murat et al., 2023), and PWR KONVOI, in the frame of doctoral thesis at KIT and the NUSAFE program.

It is worth reminding here that the calculation route in Fig. 2 has the potential to represent valid support to the emergency and decision-making teams during a hypothetical severe accident, because of the use of mature and extensively validated tools for simulating the fuel depletion (KORIGE, ORIGEN), the accident progression and source term (ASTEC), and the fission product dispersion in the environment (JRODOS).

In particular, the employment of the results from the ASTEC code as input for JRODOS evaluations is a first-of-its-kind systematic approach for improving the quality of the prediction of the radiological consequences in such abnormal accidents. Having this in mind, examples of some of the latest applications of such platform of codes is provided in the following. The ASTEC model of a generic VVER-1000 NPP and some selected source term results for a LBLOCA (850 mm on the cold leg) + SBO accident scenario have been introduced in Chapter 4. The computed source term has been employed by JRODOS to evaluate the radiological consequences to the public and the environment of the occurrence of such hypothetical accidents in one unit located in the Kozloduy NPP site (Bulgaria) (Mercan et al., 2022) in winter weather conditions. For the JRODOS calculations, an area of 1600 × 1600 km^2 has been considered and the Bulgarian criteria over sheltering, evacuation, and stable iodine distribution have been considered for the emergency actions, i.e. the sheltering becomes active for an effective dose rate larger than 10 mSv and the evacuation signal occurs when the effective dose reaches 50 mSv. The JRODOS results concerning the total aerosol deposition after 10 days from the accident are shown in Fig. 16. The results show that the cloud first is transported in the west-southwest direction from the plant site on the first day of the calculation, and then the contamination spreads to the southern regions of the selected area over the next 9 days. Due to the orography of the area, the higher deposition regions are observed in the valleys between the mountains. The results in Fig. 16 show that the highest total contamination by aerosols is about 22.9 MBq/km^2, The analyses in (Mercan et al., 2022) show that the iodine release plays a major role. The calculated maximum value of the total committed effective dose for normal living is 106 mSv in the 4 km^2 area around the site and decreases up to less than 1 mSv up to 50 km west of the site due to cloud movement. The results of the work therefore show that the conditions for local sheltering and evacuation are not reached.

Further ASTEC/JRODOS investigations have been performed for a hypothetical LBLOCA (850 mm break on the hot leg) in conjunction with an SBO located at the Akkuyu site (Turkey). Such analyses lead to different radiological consequences than in the previous case. The accident is postulated to occur in the summertime and the German regulations are considered for emergency action. Namely, the evacuation is planned to be performed when the effective dose reaches 100 mSv and the actions for temporary and permanent relocation of the population are applied when the effective dose is larger than 30 mSv and 100 mSv, respectively. The JRODOS results for the total deposition of aerosols after 10 days from the accident are shown in Fig. 17. The JRODOS

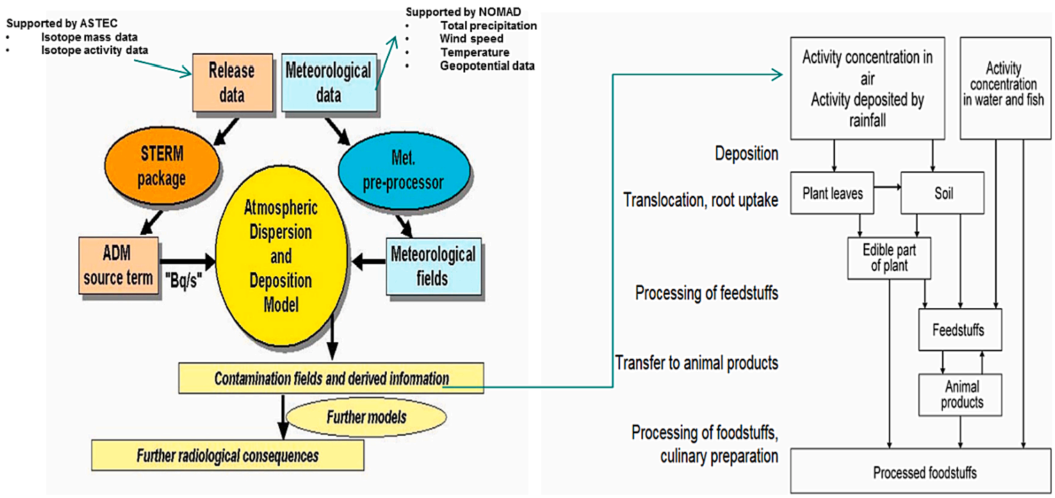


Fig. 14. Scheme of the JRODOS tool for the prediction of the radiological dispersion after a hypothetical severe accident.

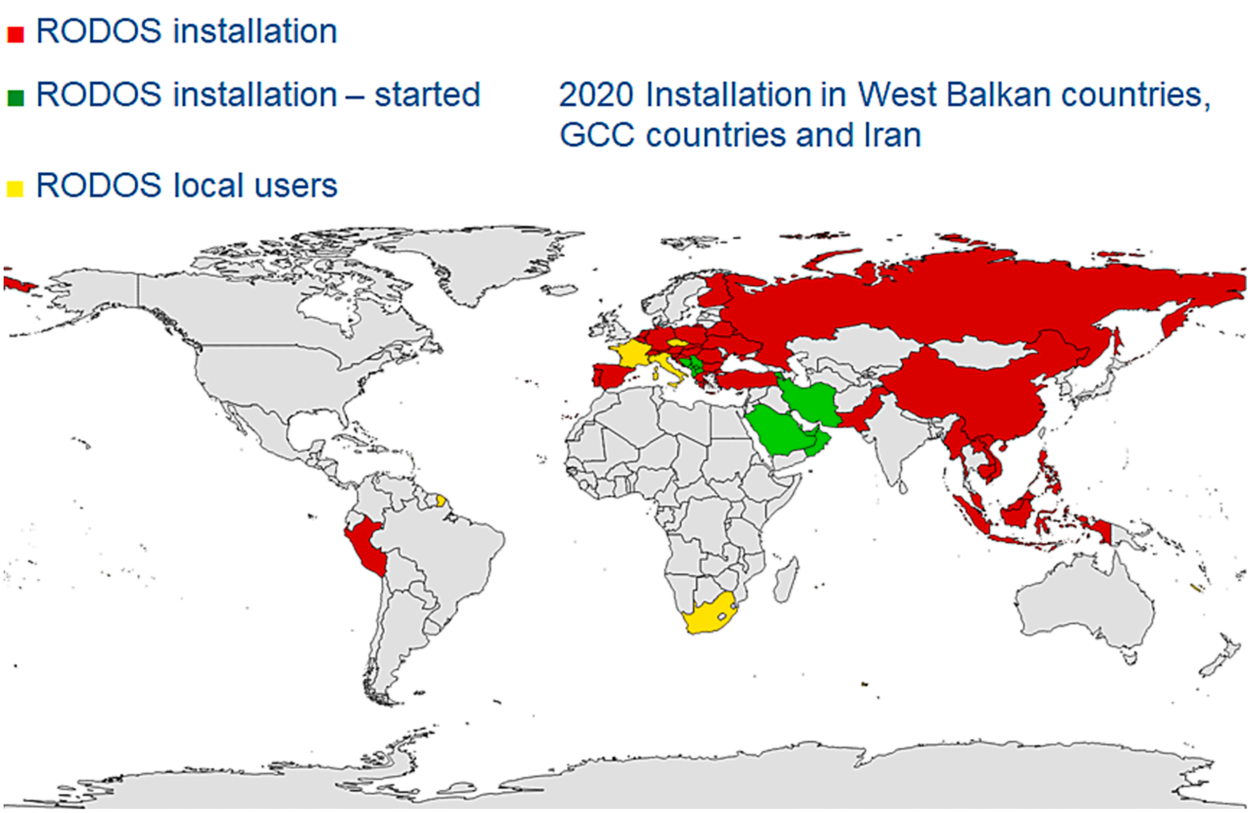


Fig. 15. Overview of users of JRODOS in the world.

predictions show that the contamination mainly spreads north and north-west part of the site on the first day of dispersion and then moves to the southeast affecting eastern Anatolia, Greece, and Cyprus. The aerosol contamination reaches about 11.5 GBq/km^2 and may be observed up to 200 km from the site. In the same area, the results for the iodine contamination may approach 0.247 GBq/km^2. As a result, the JRODOS emergency tool predicts that about 3.8 million people are needed to be sheltered and about 1.3 million people are requested to be evacuated.

ASTEC/JRODOS analyses are currently going on to evaluate the radiological consequences of a hypothetical ST-SBO of the generic Peach Bottom Unit-2 BWR introduced in Chapter 4 (Murat et al., 2023). As a preliminary analysis, the actual geographical location has been considered and a mesh grid within 400 km from the site has been modeled in JRODOS. The accident is postulated to occur in the winter time and the JRODOS simulations have been carried out to calculate the radiological consequences up to one day after the event. Furthermore, no early countermeasures have been considered by the emergency teams.

The distribution of the total effective gamma dose rate after one day from the accident is shown in Fig. 18. According to the United States regulation, the maximum limit for individual public and radiation workers in a year is 1 mSv and 5 mSv respectively (U.S. Nuclear Regulatory Commission, 1991). By comparison with such reference data, the JRODOS results show that the computed dose rate exceeds such limits. Such preliminary analysis has represented a solid basis of understanding

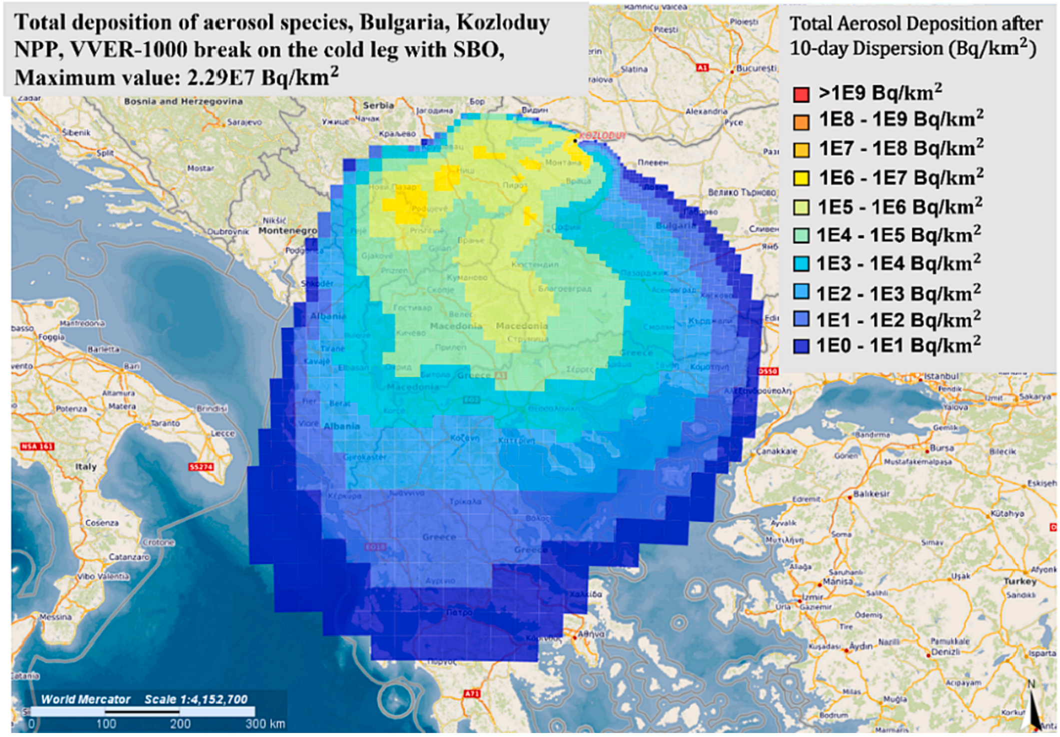


Fig. 16. Total aerosol contamination after 10 days for a hypothetical LBLOCA on the cold leg in conjunction with SBO in one unit at the Kozloduy site.

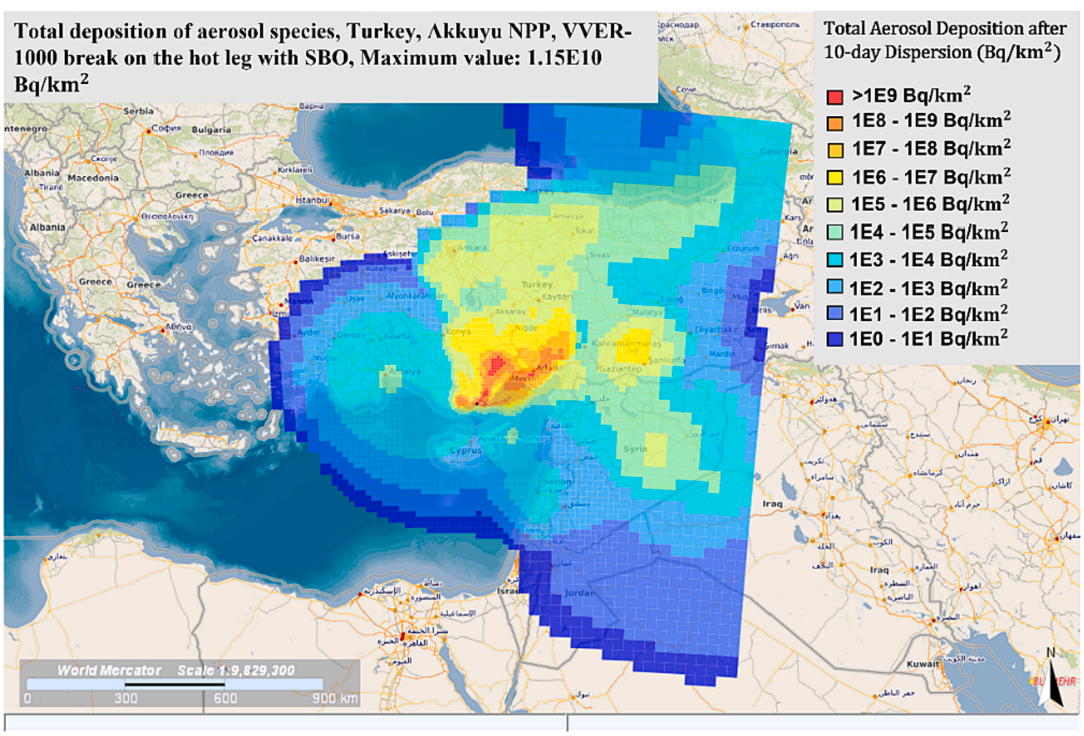


Fig. 17. Total aerosol contamination after 10 days for a hypothetical LBLOCA on the hot leg in conjunction with SBO in one unit at the Akkuyu site.

for further and more extensive ASTEC analyses for BWR NPPs, which are currently going on.

The calculation platform in Fig. 2 has been employed to compute the radiological consequences of a hypothetical MBLOCA (12′' break on the cold leg) in the generic KONVOI ASTEC model described in Chapter 4. In the JRODOS simulations, the plant is located in the Cattenom site (France), where 4 PWR-1300 Units (built between 1979 and 1991) are in operation. For such analyses, the fuel inventory at EOC, namely with the largest amount of fission products, has been employed in the ASTEC model for the evaluation of the source term. Two JRODOS simulations have been performed by using weather data for winter and summer times and the behavior of the cloud has been monitored for 10 days after the accident. The results concerning the total dose from all exposure (without ingestion) are shown in Fig. 19 and Fig. 20, for the winter and

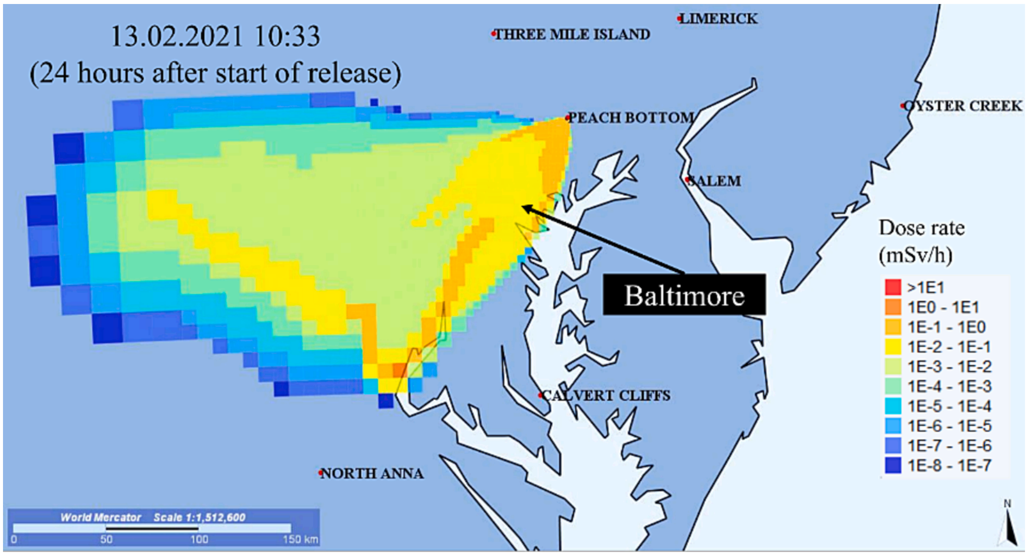


Fig. 18. Total effective gamma dose rate 24 h after a hypothetical ST-SBO accident in the Peach Bottom Unit-2 NPP.

the summertime, respectively. The results show that the maximum value of the dose is below the limits. It is worth observing that a larger area is involved when the accident occurs in the winter than in the summertime. In particular, one may observe that in the worst-case scenario, the cloud may cover the full central Europe from France to Poland. Further studies are going on at KIT to investigate the radiological consequences of other hypothetical accidents, e.g., Small Break LOCA (SBLOCA), also in conjunction with an SBO.

Finally, the application of the KORIGEN/ASTEC/JRODOS calculation platform in Fig. 2 demonstrates the current capabilities at KIT to investigate the radiological consequence of a hypothetical severe accident for any reactor, accident sequence, region, and meteorological conditions. Such capabilities represent a unique instrument available at KIT to support the emergency teams and the decision-making during hypothetical severe accidents.

6. The KArlsruhe tool for uncertainty and sensitivity analysis (KATUSA)

KATUSA code has been developed at KIT (Stakhanova et al., 2022)

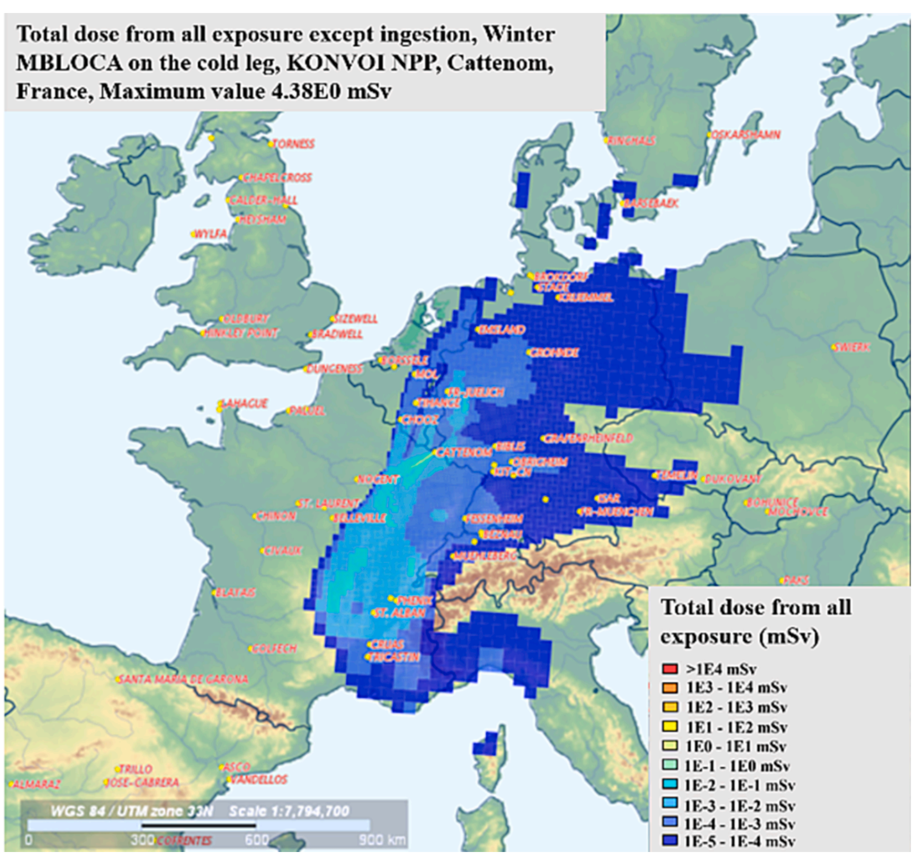


Fig. 19. Total dose from all exposure 10 days after a hypothetical MBLOCA accident in a generic KONVOI NPP at the Cattenom site. winter time.

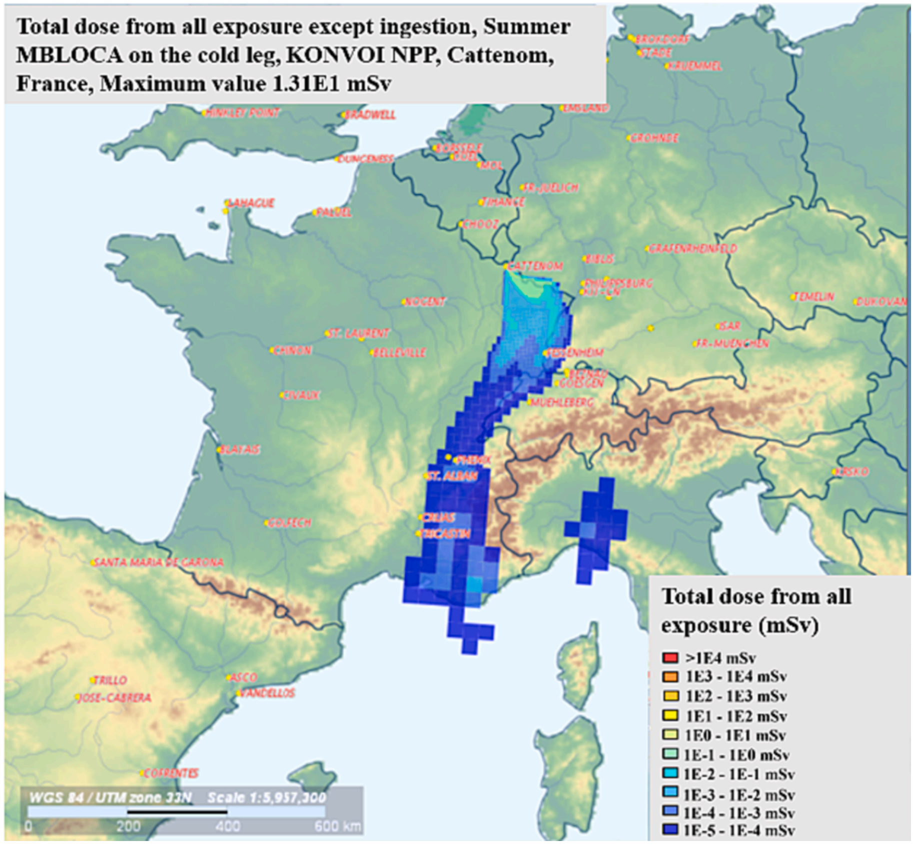


Fig. 20. Total dose from all exposure 10 days after a hypothetical MBLOCA accident in a generic KONVOI NPP at the Cattenom site. summertime.

for uncertainty and sensitivity (U&S) analysis. Initially, it was applied to do a U&S-analysis of ASTEC when predicting the radiological source term (ST). The flowchart of an ASTEC/KATUSA calculation is shown in Fig. 21. The black boxes indicate the input data provided to the calculation platform, e.g. the probability Density Function (PDF) of the uncertainty input parameters and a reference input deck. The blue boxes indicate the results of the main KATUSA modules, which are labeled by the red boxes.

To run the sampling module user specifies the uncertain input parameters, their PDFs and PDFs parameters, the number of samples, the sampling method, and whether input parameters are correlated. The "Sampling" module supports Latin Hypercube Sampling (LHS) (McKay et al., 2000) and Simple Random Sampling (SRS) algorithms. The available probability density functions are uniform, normal, truncated normal, beta, and triangular. Also, an option for discrete uncertain parameters has been added. Uncertain input parameters can be correlated, and to re-order the sampling results according to the input correlation matrix the Iman-Conover method is used (Iman and Hora, 1990). The "Run multiple simulations" module takes the results of the sampling and the input files of the selected code as input. Currently, KATUSA is coupled with the ASTEC and TPF codes. This module prepares the file with the uncertain input parameter values individually for each simulation, and it runs simulations in parallel. After all simulations are finished, it failed runs are checked. This is done by the "find samples to exclude" module. In addition, the code can check some special characteristics of the individual simulation results, like the time of the main events happening during severe accident progression in case of using the ASTEC code for simulations. This gives additional information about the influence of the input parameter changes on the output results. For this step, the user specifies the list of Figures-of-Merit (FoMs) and runs the "collect data" module. This module extracts the data of specified parameters from all simulations for the whole time scale. The collected

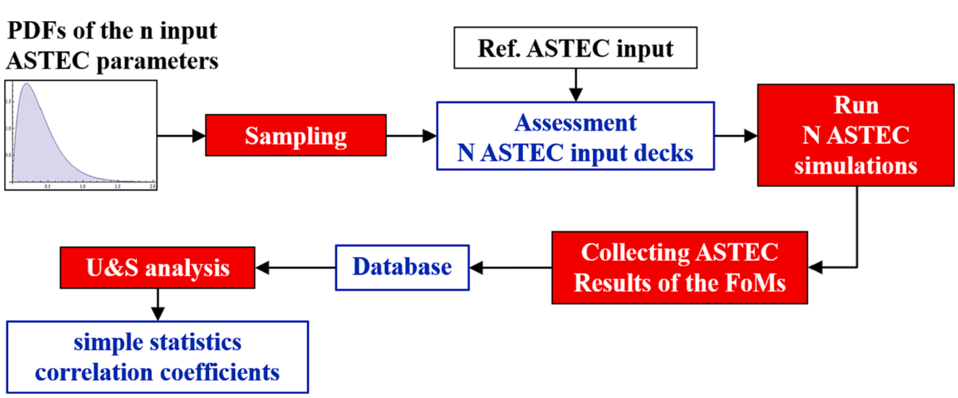


Fig. 21. The KATUSA workflow and main modules.

data are stored in the databases. Now the user can decide about the time window for further U&S analysis. To do so the two time points can be specified in the input file or, in the case of the ASTEC code, it can be the name of two events happening during the SA progression (for example, the user can take only the data between the start of fission products release and the lower head vessel failure). In the input file of the "filter data" module the user can shorten the list of FoMs if needed, by default all FoMs from the previous step will be considered. For each simulation the data is extracted between two selected points, and after that interpolated on the one-time scale. The interpolated data is again stored in the databases.

Finally, everything is prepared for U&S analysis itself. The user decides whether to calculate the simple statistics and which correlations are required. Also, the list of FoMs can be shortened again, or by default, all FoMs from the previous step are considered. The available correlations are Pearson, Spearman, distance (Martinez-Gomez et al., 2014), and maximal information coefficient (Kinney and Atwal, 2014). The "U&S analysis" module creates plots with simple statistics and correlation values for all FoMs and these data are stored in the databases for further use. KATUSA can be used for uncertainty quantification and sensitivity analysis of different solvers such as SCF, TPF, PARAFISH, TRACE, and PARCS. In addition, a Graphical User Interface (GUI) is under development to make it more user-friendly.

KATUSA has been extensively employed at KIT to perform the U&S analysis of the ASTEC source term results for selected severe accident sequences in the generic KONVOI NPP introduced in Chapter 4 in the framework of the joint KIT and Framatome participation to the MUSA project (Herranz et al., 2021). Having this in mind, the ASTEC/KATUSA platform shown in Fig. 21 has been employed to quantify the uncertainty of the amount of key fission products, i.e. Xe, I, and Cs, in the containment and released to the environment during selected scenarios as well as the evaluation of the correlation coefficients, i.e. Pearson and Spearman, of selected ASTEC uncertainty input parameters on such FoMs. Efforts have been spent to identify 16 uncertainty parameters and to assess the corresponding PDFs based on literature review and engineering judgments. The selected uncertainty parameters are employed in ASTEC to model key phenomena affecting the source term, namely the fission product released from the fuel, the cladding integrity criteria, the properties and the behavior of the aerosols, the initial fuel inventory, and the containment leakage.

As an example of the application of the ASTEC/KATUSA platform, results for a hypothetical severe accident initiated by a MBLOCA (12'' on the cold leg) are discussed here. The following FoMs are analyzed in the study: the amount of Xe and I and Cs aerosols in the containment and of Xe, I, and Cs released to the environment as the fraction of the initial loading. For such investigations, 300 ASTEC simulations were run and the LHS was employed to propagate the uncertainties of the input parameters to feed the database for performing the U&S analysis. It is worth noting that less than 5% of the runs failed, namely the ASTEC code looked rather robust. The simple statistics of the results concerning the amount of Xe are shown in Fig. 22. Since, as expected, almost all the Xe loaded in the core is released to the containment, the mean value approaches the 95% value, which is very close to the maximum. Concerning the environment, the mean value and the 95th percentile at the end of the last instant considered in the database are about 2% and 3.2% of the initial loading, respectively. The results concerning the I-aerosols in the containment and the total I release to the environment are shown in Fig. 23. It may be observed that the mean value of the amount of I aerosols in the containment (Fig. 23, left) reaches up to about 1% of the initial loading and the 95th percentile up to about 10%. Concerning the environment (Fig. 23, right), the mean value and the 95th percentile are about 0.005% and 0.02% of the initial loading, respectively. The results concerning the Cs aerosols in the containment and the total I release to the environment are shown in Fig. 24. The results show that the mean value of the Cs aerosols in the containment approaches 5% of the initial loading and the mass fraction is below 10% in 95% of the samples (Fig. 24, left). Concerning the environment, the mean value and the 95th percentile are about 0.015% and 0.035% of the initial loading, respectively (Fig. 24, right).

ASTEC databases for performing U&S analysis have been assessed not only for the KONVOI but also for VVER-1000 and GE-BWR NPPs and are continuously fed by implementing the results for different scenarios. Such activity is performed in line with the KIT strategy discussed above and aims at two main goals: supporting the improvement of the performance of the ASTEC code and quantifying the uncertainty of the source term given the JRODOS analysis. Extensive sensitivity analysis has the potential to identify the input parameters and physical models for which more efforts have to be spent to reduce their uncertainty. At the same time, the uncertainty quantification of the source term is a key issue to further improve the current capabilities to predict the radiological impact of a hypothetical severe accident and then to support the emergency teams.

7. KIT multi-physics coupling codes for improved core analysis

For consideration of cross flow between fuel assemblies in the case of fuel-assembly-based simulations or between the sub-channels in the case of pin-based simulations, SCF was coupled with different solvers, COBAYA3 (Calleja et al., 2014), DYN3D and CRONOS (Jimenez, 2015), in the European simulation platform NURESIM. It was also coupled with the DYN3D-MG version (multi-group diffusion) and DYN3D-SP3 (simplified transport SP3) for fuel-assembly- and pin-based simulations of reactor cores (Daeubler et al., 2015). A coupling of SCF code with the core simulator PARCS is also under testing and validation (Basualdo and Sanchez, PARCS/Subchanflow: Nodal Internal Coupling, 2015). A comparison of the total power predicted by COBAYA3/SCF for

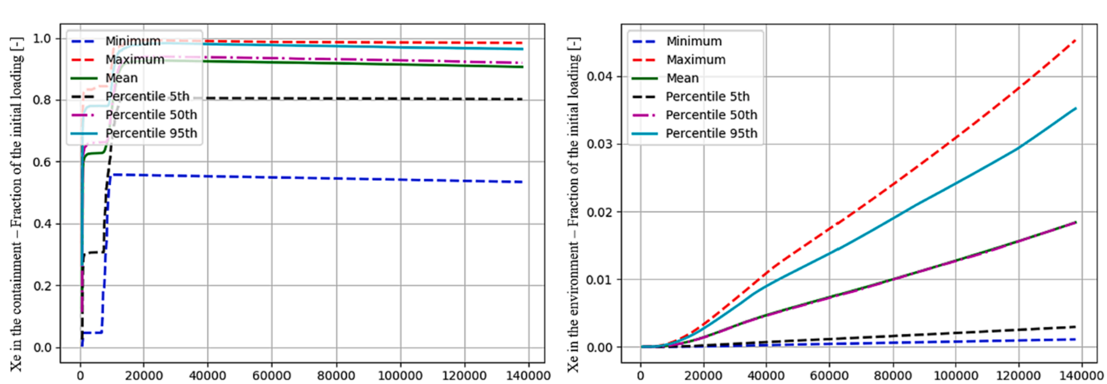


Fig. 22. Simple statistics of the mass of Xe in the containment (left) and in the environment (right) as the fraction of the total amount in the initial core loading in the ASTEC MBLOCA scenarios.

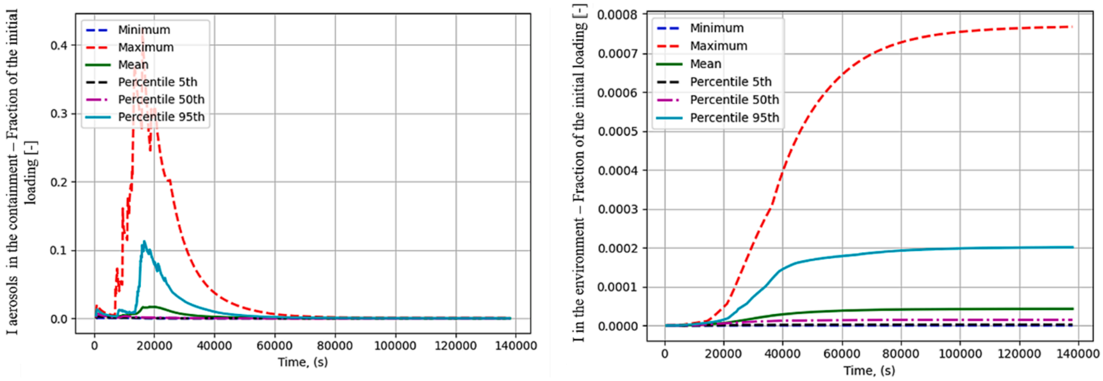


Fig. 23. Simple statistics of the mass of I aerosols in the containment (left) and of the total mass of I in the environment (right) as the fraction of the initial core loading in the ASTEC MBLOCA scenarios.

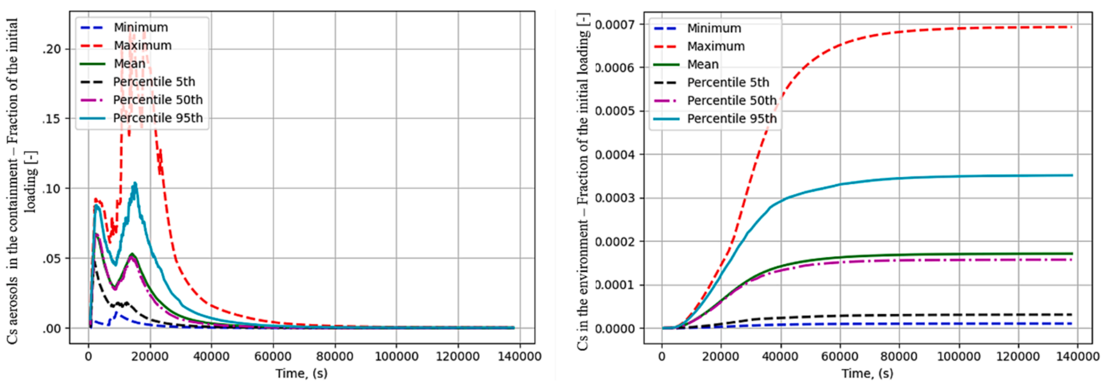


Fig. 24. Simple statistics of the mass of Cs aerosols in the containment (left) and of the total mass of Cs in the environment (right) as the fraction of the initial core loading in the ASTEC MBLOCA scenarios.

the transient "switch-off of one of the four Main Coolant Pump (MCP)" of a VVER-1000 reactor and the measured data is presented in (Calleja, 2013). The SCF model consisted of one channel per fuel assembly where the cross-flow is permitted between FAs, i.e. it was a 1-to-1 radial mapping between neutronic (N) and TH (TH) domains. It can be observed that the code predictions are close to the measured ones (Neutron Flux Control (NFC) and Self-powered Neutron Detector (SPND)).

7.1. Nodal diffusion solvers coupled with subchannel codes using ICoCo

- **The coupled code PARCS/SCF based on ICoCo**

The nodal diffusion solver PARCS is coupled with both the internal coupling approach (Basualdo and Sanchez, 2015) and the ICoCo-based approach. Latter is very flexible and it allows the coupling at pin/sub-channel and fuel-assembly/channel levels based on the mesh-to-mesh superposition (Garcia, 2021). The coupling between PARCS and SCF has been implemented at KIT through the ICoCo interface (CEA, 2021). The main advantage of this coupling approach is that it does not interfere with the syntax of the codes, i.e. inputs have to be made for PARCS and SCF as usual. A MED mesh, as available in the SALOME platform is generated using a MED pre-processor (Garcia, 2021), for the codes to store the variables fields, and, via ICoCo routines, both codes communicate using get and set functions for fields and time step definition.

The PARCS/SCF-ICoCo is currently being used within the framework of the EU2020 MCSAFER Project, which focuses on SMR concepts. Specifically, the Korean SMART and Argentinian CAREM concepts were studied under postulated transient scenarios using the coupled tool. The results have been compared against other coupled tools used by partners of the project, and have shown good agreement. Detailed information on this work can be found in (Fridman et al., 2022).

- **The coupled code PARCS/TPF/ICoCo**

The neutronic/TH coupling between PARCS and TPF can be seen from two perspectives. From the computer science perspective: since the ICoCo approach was followed, the coupling of PARCS and TPF is external. The codes are executed in a serial process by a third-party program, called *Supervisor*. From the mathematics perspective: the Supervisor orchestrates the data exchange using *MEDCoupling* library functions; for this purpose, MED format meshes were created for each code, as well as the ICoCo methods for initialization, time advance, and field exchange were integrated into PARCS and TPF is sketched in Fig. 25.

The domain of both codes is overlapped, and node-wise data is mapped from mesh to mesh. Last, an explicit iterative process for data transfer was chosen. Exchange variables are power, fuel temperature, coolant temperature, and coolant density. Fig. 26 shows the iterative process for PARCS/TPF coupled calculation. For steady-state calculation, PARCS calculates the first step assuming initial TH parameters, and then the predicted power is transferred to TPF. With the new 3D power distribution TPF predicts the T/H feedback parameters and transfers them to PARCS. Then, a new steady-state iteration step is done, this iterative process is executed until convergence criteria are met. The

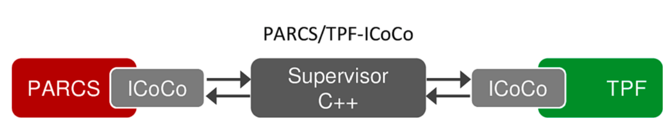


Fig. 25. PARCS/TPF coupling based on ICoCo-Interface.

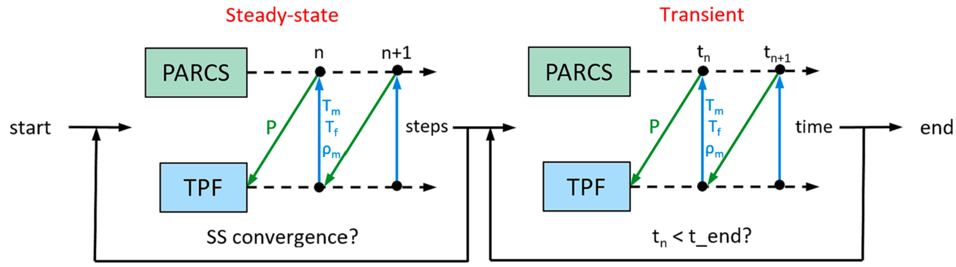


Fig. 26. PARCS/TPF iterative scheme for coupled calculation.

transient calculation starts with the steady-state converged solution. Similarly to the steady-state iterations, data is transferred each time step, the transient continues until the end time is reached. For the transient calculation, both codes use the same time step, this time step is set as the smallest of the internal time step of each code as presented in Fig. 26.

The verification of the coupling of TPF with PARCS is being performed by a code-to-code comparison with the results obtained by the coupled code PARCS/SCF for the KSMR Rod Ejection Accident (REA). In Fig. 27, the comparison of the total power and reactivity evolution after an REA at Hot Zero Power (HZP) conditions is shown (top: left and right) as well as the maximal fuel and coolant temperature (left bottom) as well as the 3D fuel assembly radial power distribution (right bottom) as predicted by the two coupled codes PARCS/SCF and PARCS/TPF.

A very good agreement of the global parameters (power and reactivity) is achieved by the two codes and a small deviation of the fuel temperature is predicted, where SCF tends to slightly over-predict the fuel temperature. The reasons for this may be the differences in the heat transfer correlations implemented in both TH codes.

7.2. *ICoCo-based coupling of diffusion solvers with subchannel code at pin/subchannel level*

The code applied in this section inherits substantially from the code described in section 7.1, with two major developments to PARCS and the Cross Section (XS) generation:

1) Enable PARCS to be able to process "big cases" (reflected by the big matrix e.g. pin level fuel and control rod arrangement in PARCS normal inputs) with diffusion nodal solvers;
2) Optimize the pin-level XS generated by the Monte Carlo code Serpent for PARCS with the Super-Homogenization (SPH) method (Hébert and Kavenoky, 1981) to improve the prediction of PARCS with the diffusion nodal solver.

The first development touches the PARCS source code while the second develops an optimization system based on Python. Especially, within the SPH system, PARCS runs iteratively to approach the Serpent solution with iteratively-optimized XS. The overall execution scheme is given in Fig. 28.

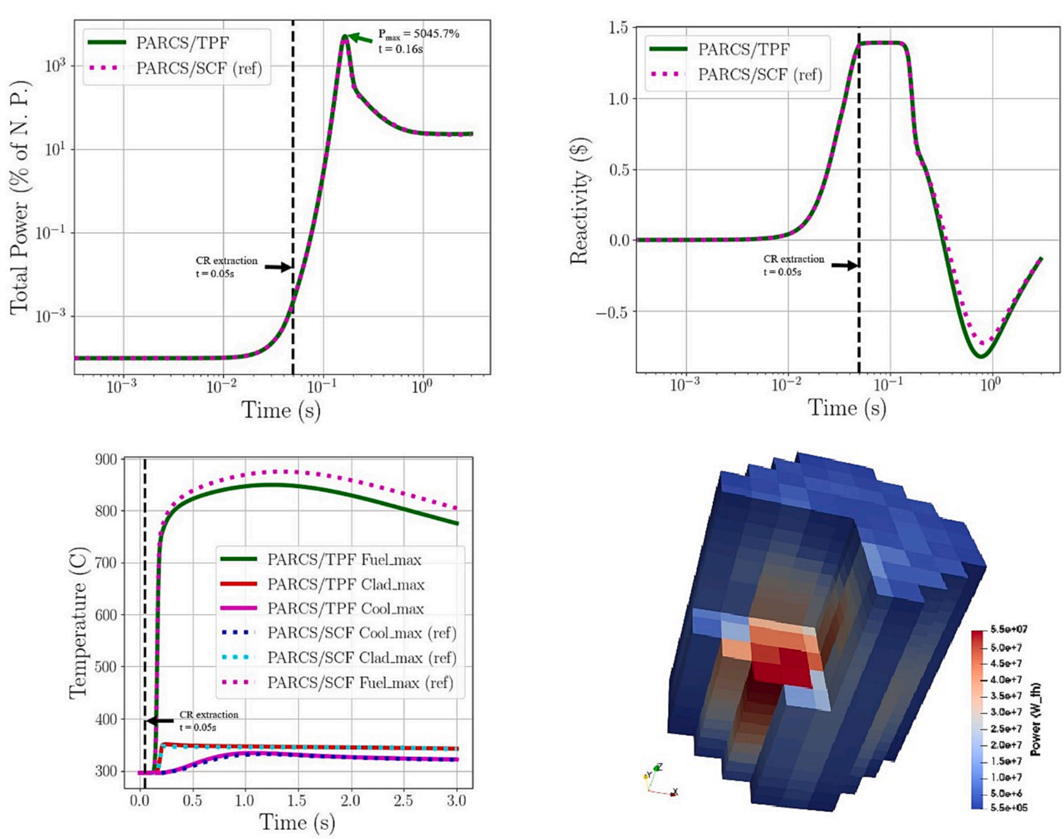


Fig. 27. PARCS/TPF results for the KSMR REA analysis with PARCS/TPF compared to the ones of PARCS/SCF.

The code along with the XS optimization system was used to perform a pin-level simulation for the KSMR core (an academic SMR based on the Korea SMART concept). Two scenarios were considered: a) steady state with all control rods out; b) transient of a REA. Details of the operation conditions and transient sequence can be found in (Alzaben, 2019). Fig. 29 and Fig. 30 present some selected primary results to demonstrate the code's capability on pin-level simulations.

It is worth noting that the current pin-level simulation uses the traditional nodal solver and is only possible with the PARCS diffusion solver. Pin-level models of the KSMR core for the PARCS Fine Mesh Finite Difference (FMFD) solver (there, SP3 is available) are now under development at KIT and will be applied to the coupled code PARCS/SCF-ICoCo. Along with the XS optimization system, this SP3-based pin-level multi-physics coupling system will be verified.

7.3. Internal coupling of the nodal diffusion solver with subchannel thermal hydraulics and thermo-mechanic solvers (PARCS/SCF/TU)

The coupled code PARCS/SCF was extended by the inclusion of the thermo-mechanics code named Transuranus (TU) for a more realistic prediction of the behavior of irradiated fuel rods. An internal coupling of PARCS/SCF/TU was developed with an MPI-parallel capability to simulate the behavior of LWR cores describing the thermo-mechanics behavior in a more precise manner by TU (Basualdo et al., 2017; Basualdo et al., 2018). In this approach, the fuel rod model of SCF is replaced by the more precise TU-code. Since TU can predict only one representative fuel assembly, single TU inputs are generated in separate folders as many fuel assemblies exist in the core. In a pre-step, single TU burn-up simulations are performed for each fuel assembly until the desired burn-up of fuel assembly that corresponds to the core loading is achieved. The transient coupled simulation of an REA is started with a coupled executable of the three codes. Then, e.g. 193 MPI processes are started for TU. At each time advancement, the feedback between the neutronics and the THs and thermo-mechanics are exchanged in the MPI-framework until the problem time is achieved. In Fig. 31 (left), the 3D enthalpy distributions added to the core at 1 s transient time as predicted by the coupled code is shown. There, on the right side, the difference between the axial heat transfer coefficient and the gap width as predicted by PARCS/SCF/TU for a fresh and a burnt core (FA number 160) is shown. It can be seen that the Heat Transfer Coefficient (HTC) and the gap width vary considerably along the core height for the burnt FA.

7.4. Internal coupling of SP3-solver with subchannel codes

Parallel to the coupling of Monte Carlo codes with subchannel codes, the DYNSUB5 code was developed. It consists of the internal coupling of DYN3D-MG (multi-group diffusion and SP3 solver) with Subchanflow for improved LWR core analysis at pin /subchannel level (Gomez-Torres et al., 2012; Daeubler et al., 2015). This coupling code can perform steady state and transient solutions at pin/fuel assembly using the SP3 or multi-group diffusion approximation considering local feedback. An explicit marching iterative scheme is implemented between the neutronic and TH solvers. To speed-up the solution of large problems, e.g. a PWR core, a relaxed Picard iteration is implemented. A flexible axial and radial mapping of both computational domains was implemented, too. XS libraries are generated using the SCALE6 or Serpent2 codes using the in-house tool (createXSlib) in dependence on the TH conditions. It also includes corrections for the pin cell homogenization procedure e.g. SPH for pin-by-pin diffusion or SP3 core simulations and IDF-correction for the pin-by-pin or nodal diffusion solution (Daeubler et al., Generation and application of interface discontinuity factors in the reactor simulator DYN3D, 2014). The unique capabilities of the DYNSUB5 code were demonstrated by analyzing a rod ejection accident of a PWR core defined in the PPWR UOX/MOX benchmark (Kozlowski and Downar, 2003).

7.5. High-fidelity Monte Carlo codes coupled with subchannel codes

7.5.1. Steady-state core analysis at pin/subchannel level with coupled Monte Carlo and subchannel codes (MCNP5/SCF, Serpent2/SCF)

At KIT different coupling approaches were developed between subchannel codes and different Monte Carlo codes such as MCNP5 and Serpent2. First, these codes were internally coupled with the in-house SCF for pin/subchannel level analysis of the PWR core (Ivanov et al., 2014) and (Daeubler et al., 2015). These developments paved the way for very detailed simulations of full PWR cores to provide reference solutions for any low-order neutronic/TH-coupled simulation for which no experimental data is available. In (Daeubler et al., 2015), the 3D distribution of the pin power in the PWR UOX/MOX core predicted by Serpent2/SCF is shown for Hot Full Power (HFP) conditions. The critical born search simulation using 2048 cores needed around 1.03 days to get a converged solution. This kind of tool allows the direct prediction of local safety parameters in a direct manner. The first validation of MC/TH coupled codes was done using the data of the MIT PWR BEAVRS benchmark (Horelik et al., 2013) at hot zero power conditions, e.g. data of eigenvalue, control rod worth values, assembly power for different positions, was made available.

7.5.2. Depletion analysis of LWR cores with coupled neutronic, TH, and thermo-mechanic codes (Serpent2/SCF/TU) at pin/subchannel level

Within the framework of the recent EU McSAFE Project (Sanchez et al., 2021), KIT developed new coupling approaches for the Serpent2, SCF, and TU codes based on the ICoCo interface (Garcia et al., 2020), as presented in Fig. 32. These new advanced coupling schemes allow for an improved description of the fuel behavior of modern core loadings during reactor operation (i.e. the depletion of the fuel), allowing the prediction of burn-up-dependent safety parameters for LWRs. The data transfer between the different physic domains is performed by a mesh-to-mesh superposition with the powerful MEDcoupling library. A C++ program acts as supervisor and it controls the call of each solver as well as the time advancement. The semi-implicit burnup scheme implanted for fully coupled simulations of the core neutronics, depletion, THs, and thermo-mechanics is shown in Fig. 32. According to this approach, the SCF fuel rod solver is replaced by the more sophisticated one available in TU. Also, in this scheme, a detailed depletion is carried out by Serpent2

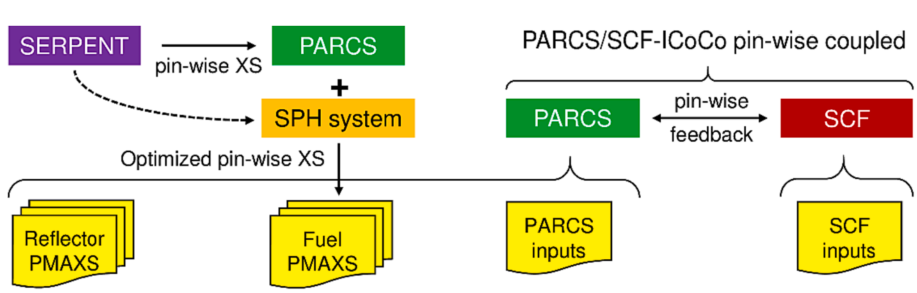


Fig. 28. Pin-level execution scheme of the ICoCo-based coupling code PARCS/SCF with the XS optimization.

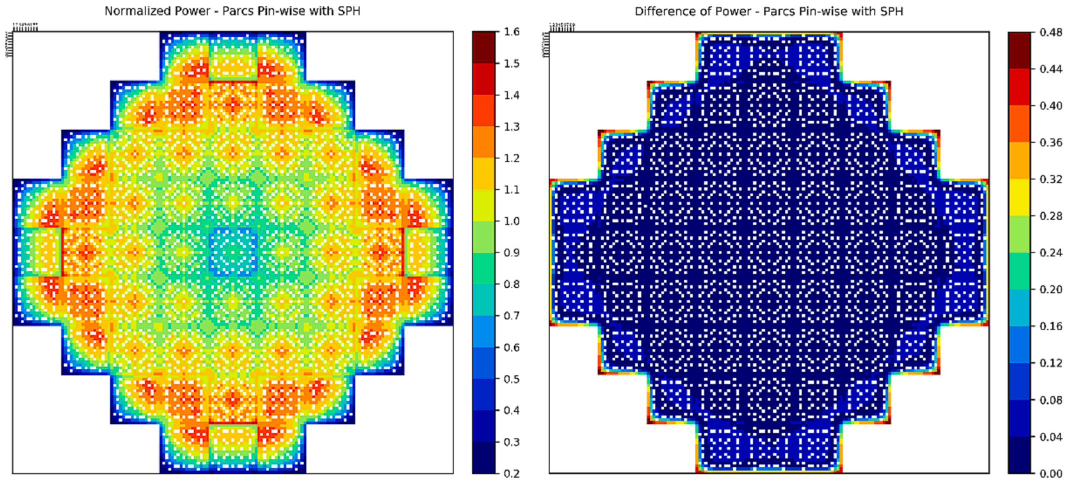


Fig. 29. The distribution of axially-averaged relative power (left) and the result difference compared with Serpent (right).

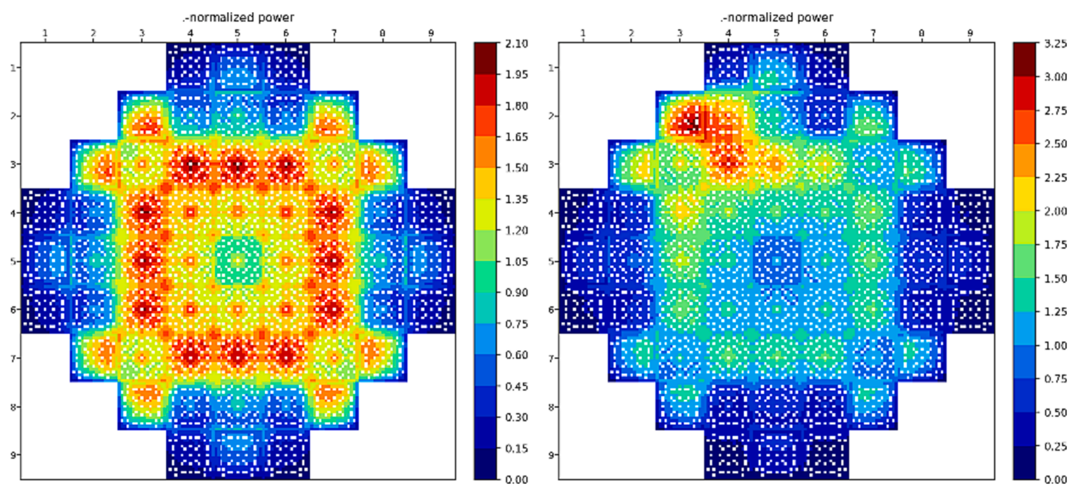


Fig. 30. The distribution of axially-averaged relative power at the beginning of the transient 0.0 s (left) and at the peak power time 1.4 s (right).

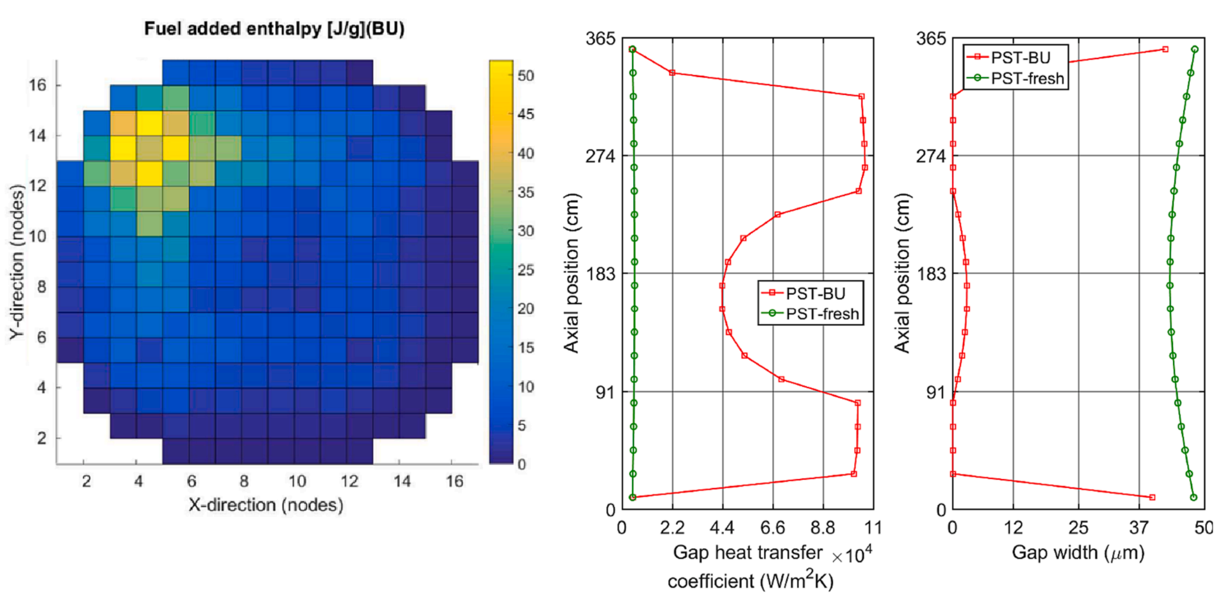


Fig. 31. Analysis of a UOX/MOX REA with PARCS/Subchanflow/Transuranus; left. 3D fuel enthalpy added to the core during the REA at 1 s transient time, Axial gap HTC and gap width predicted for the fuel assembly number 160 for a fresh and burn core loading (right). Large differences of the HTC and gap width exist (Basualdo et al., 2018).

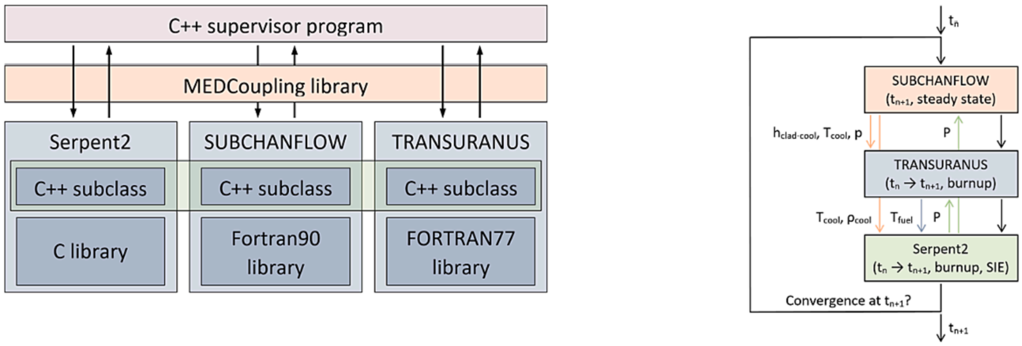


Fig. 32. Object-oriented coupling approach (right) based on ICoCo between Serpent2/Subchanflow and Transuranus for improved depletion simulations of LWR-core loadings [MG] and the semi-implicit burn-up scheme implemented (Garcia et al., 2020).

code, while a simplified one is done by TU. To enable the memory scalability needed for these massive problems, a Collision-based Domain Decomposition (CDD) scheme has also been implemented in Serpent 2 (García et al., 2021). The methodology is based on data decomposition for burnable materials and a domain decomposition particle-tracking algorithm and was proved to provide the required memory scalability and computational performance, with up to 50% speedup efficiency at 5,120 cores. This powerful coupling approach paved the way for detailed full core analyses at the pin/subchannel level with depletion capabilities and was validated using plant data from the German KONVOI PWR plant and from the VVER-1000 Temelin-2 plant (García et al., 2021) and (García et al., 2021). Very good agreement was obtained for key-parameters (e.g. for the boron concentration, the local axial power distributions, and radial fluxes) between the measured data and the prediction with Serpent2/SCF/TU.

The coupled codes Serpent/SCF and Serpent/SCF/TU were validated using measured data (boron concentrations, neutron flux) of the German PWR pre-KONVOI and data of the VVER-1000 Temelin plant obtaining were good results i.e. the experimental data falls within the statistical range of the results and no significant differences are observed between the calculations with/without Transuranus (García et al., 2021; García et al., 2021).

7.5.3. *Transient core analysis with coupled code Serpent2/SCF at pin/subchannel level*

Recent developments in the frame of different European projects such as HPMC (Hoogenboom and Sjenitzer, 2013), and McSAFE (Ferraro et al., 2018) were focused on the coupling of the Serpent2 code extended with dynamic capability i.e. for the description of the prompt and delay neutrons as well as the control rod movements with the SCF code to simulate short transients such as the REA in a PWR core. This coupling approach was based on an internal master/slave approach, where some elements of the ICoCo approach were used (Ferraro, Monte Carlo-based multi-physics analysis for transients in Light Water Reactors, 2021). The prediction capability of the first-of-the-kind coupled code Serpent2/SCF was successfully validated using the data of the unique SPERT IV REA tests (Ferraro et al., 2020), obtaining very good results for key parameters such as power increase and reactivity insertion during the REA, see Fig. 33. The error bars shown there correspond to a statistical uncertainty for the coupled simulation of a statistical error of 2 σ. It is the first validation of the dynamic capability of Serpent2/SCF using experimental data obtained in an experimental reactor.

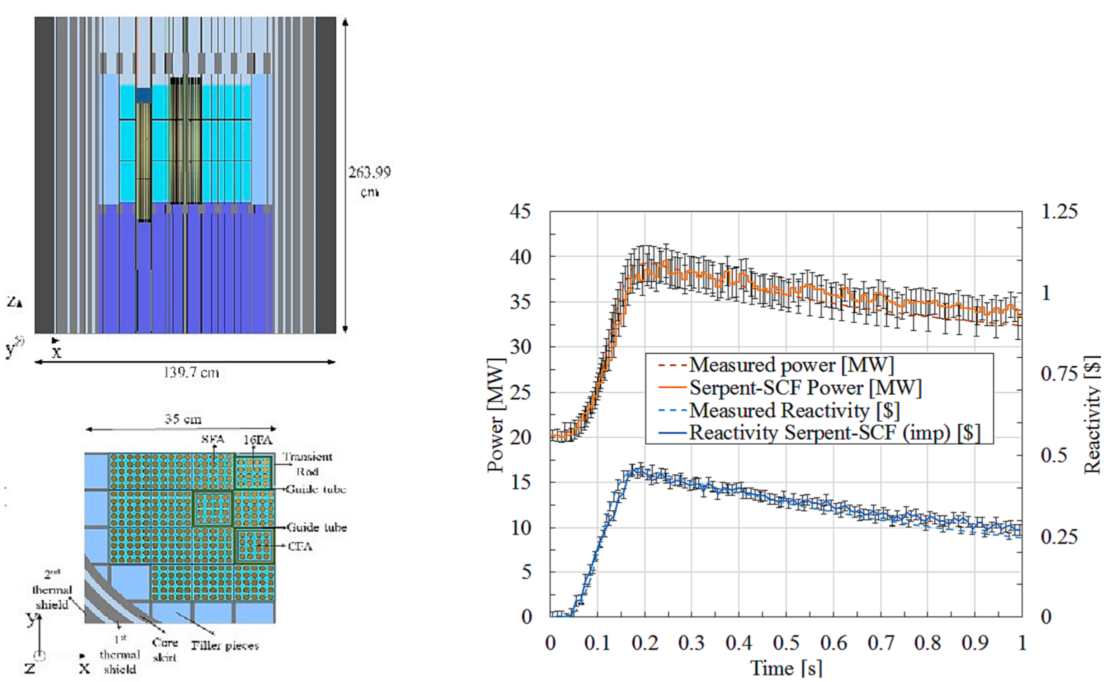


Fig. 33. Left. SPERT/IV REA core arrangement with the location of the transient rod; right. comparison of the reactor power and total reactivity evolution as predicted by Serpent2/SCF during extraction of the transient rod withdrawal for Test 84 compared to the measured data (Ferraro et al., 2020).

The high-fidelity coupling tool Serpent2/SCF is currently being used in the context of the EU2020 McSAFER and CAMIVVER projects, which focus on SMRs and VVER designs, respectively. In the McSAFER Project, a prompt-critical rod ejection transient was studied in the SMR SMART concept. A detailed 3D pin-by-pin model was developed, comprising up to 16,473 fuel pins coupled with 18,468 sub-channels for core TH. Detailed information such as coolant and fuel temperature maps can be obtained, as well as safety parameters like DNB ratio, as illustrated in Fig. 34, Fig. 35, and Fig. 36. In the CAMIVVER project, a mini-core consisting of seven fuel assemblies, derived from the specifications of the Khmelnitsky-2 VVER-1000 benchmark, was analyzed and considered as the reference solution for verification purposes within the project.

8. KIT multi-scale/-physics coupling for improved nuclear power plant analysis

Unlike the multi-physics simulation that considers multiple physical models, the multi-scale simulation focuses on the TH at different spatial scales. Considering a generic system that includes a system code (macroscale or system scale), a subchannel code (mesoscale or component scale), and a CFD code (microscale) for instance, the system code can efficiently catch the macroscopic dynamics of the entire nuclear system with coarse mesh, while the subchannel code and CFD code can particularly concentrate on the core TH and local TH details of some special part (e.g. the downcomer), respectively. The codes benefit from each other by dynamically updating their boundary conditions from other codes. In (Sanchez-Espinoza et al., 2023) a comprehensive summary of the multi-scale coupling approaches and simulations performed at KIT is provided. The following subsections overview those activities in sequence.

8.1. *Coupling of system thermal hydraulic codes with subchannel codes*

TRACE and SCF are the two TH codes that are involved in the first attempts to develop multi-scale TH coupling systems at KIT, which include:

1) The external coupling of TRACE and SCF, based on the U.S. NRC coupling interface - Exterior Communication Interfaces (ECI) (Zhang and Sanchez-Espinoza, 2019) and (Zhang and Sanchez-Espinoza, 2019, https://doi.org/10.1016/j.nucengdes.2019.110238).
2) The ICoCo-based coupling of TRACE and SCF in the SALOME platform (Zhang et al., 2021) and (Zhang et al., 2019).

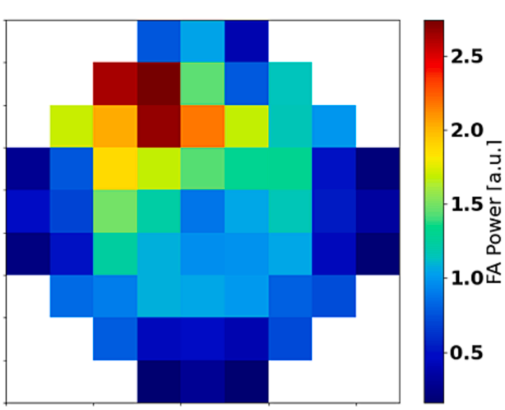
Within the ECI coupling framework (Fig. 37), the codes communicate via SOCKET, which is the basic unit of network communication. Furthermore, this is a server-less system where each involved code can directly talk with each other without a supervisor. There, SCF models the core while TRACE models other parts e.g. the RPV excluding the core (known as the domain decomposition coupling method). They run in parallel exchanging 2D data e.g. coolant mass flow rate, temperature, pressure, and boron concentration at the core inlet and outlet. The field translation between different meshes of the two codes is handled by a specially developed toolkit. Additional techniques, known as the timestep-stagged method are developed to accelerate the execution speed of the coupled code. The explicit coupling methodology was adopted for the temporal coupling.

Within the ICoCo coupling framework (Fig. 38), the SALOME platform's role is to supervise the code's execution, with a set of powerful and more user-friendly GUI toolkits. According to ICoCo standards, TRACE and SCF decomposed into several basic functional modules e.g. setDataFile and solveTimeStep, etc. Explicit meshes for the RPV and the core are developed as well for the two codes to take advantage of the MEDCoupling library (originally published with the SALOME platform) (MED, 2019) to exchange the coupled fields. There, the exchanged fields could be either 2D or 3D, corresponding to the domain decomposition (as the ECI-based coupling) and the domain overlapping coupling methods. Especially, a Dynamic Implicit Additional Source (DIAS) method (Zhang and Sanchez-Espinoza, 2019, https://doi.org/10.1016/j.ijheatmasstransfer.2019.118987) was developed to make the domain overlapping coupling possible. The two codes are explicitly coupled from the perspective of temporal coupling.

To provide the readers with a general and intuitive image of the coupling methodologies, the following two figures (Fig. 39 and Fig. 40) which include elemental concepts including the transferred data, the field translation, the meshes, and the execution procedures are given. Please note that for SALOME and ICoCo coupling, only the domain overlapping workflow is demonstrated to ease the comprehension burden of the readers. The models are for a VVER-1000 reactor.

Based on the previous two works, the coupling between TRACE and SCF now is evolving to be based on a more generic and flexible architecture, under the Europe McSafer project (Sanchez-Espinoza et al., 2021). Fig. 41 gives the draft. It is based on ICoCo as well, but a C++ script was used to replace the SALOME platform as the supervisor. TRACE and SCF run in parallel and exchange 2D fields with explicit meshes (translated by MEDCoupling) between different domains (the same as the ECI-based coupling, Fig. 39). The two codes can exchange data one time each timestep or iterate with each other within a timestep until the solutions converge, reflecting explicit and semi-implicit coupling respectively.

The motivation to adopt the straightforward coupling methods e.g. domain decomposition approach and C++ supervisor is to make the coupling system flexible and extensible to include more solvers e.g.



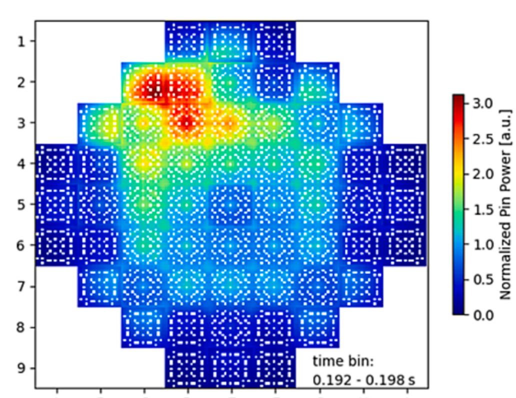


Fig. 34. PARCS/SCF-ICoCo and SERPENT2/SCF axially integrated peak power map for the prompt critical rod ejection transient scenario in the SMART concept. In this scenario, the control rod in the D2 position was ejected in 0.05 s from fully inserted to the fully extracted position.

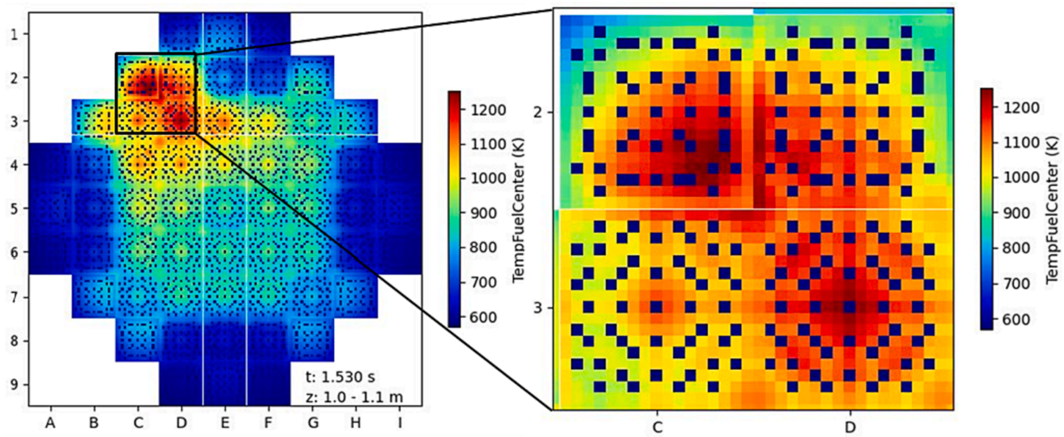


Fig. 35. Fuel centerline temperature distribution in the middle plane of the core. The left image shows the SMART full core temperature map, while the right image zooms in on the four fuel assemblies in the hot spot near the ejected control rod position.

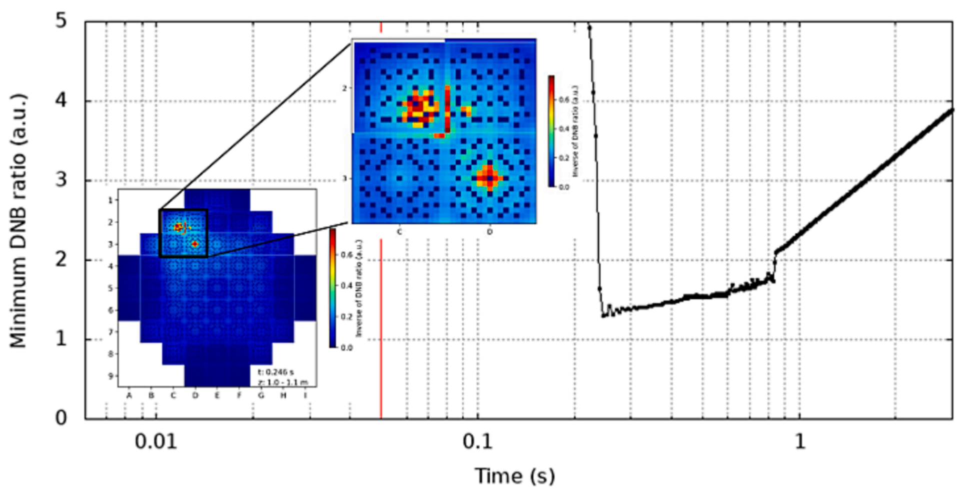


Fig. 36. The distribution of axially-averaged relative power at the beginning of the transient 0.0 s (top) and at the peak power time 1.4 s (bottom).

Fig. 37. The ECI-based coupling code TRACE/SCF-ECI.

Fig. 38. The ICoCo-based coupling code TRACE/SCF-ICoCo on the SALOME platform.

neutronic and fuel mechanic codes into the system. This is from the perspective of developing a general, flexible, and powerful multi-scale multi-physics coupling platform for nuclear safety analysis. Indeed, PARCS was implemented into this platform and coupled with SCF via ICoCo. Together with TRACE, the system TH, the core TH, and the core neutronics now can interact with each other to make the simulation closer to reality, Fig. 42.

8.2. Coupling of subchannel code with CFD code

The first CFD-involved multi-scale coupling code developed at KIT is SCF/TrioCFD. TrioCFD is an open-source CFD code based on the TRUST platform (TRio_U Software for Thermo-hydraulics) being developed by the Thermo-hydraulics Service and Fluid Mechanics (STMF) of the Department of Nuclear Energy at the CEA. ICoCo is the interface adopted by this coupling system. TrioCFD has a built-in ICoCo interface that is officially published with TrioCFD. This is exactly the reason why we select TrioCFD as the CFD code to be coupled. Similar to the previous coupled codes, its overall structure is given in Fig. 43.

The coupled codes are supervised by a C++ script that utilizes the MPI protocol and runs in parallel, explicitly. The coupled system inherently adopts the domain decomposition approach where the two codes exchange data at either the core inlet or outlet. In such cases, TrioCFD is supposed to simulate either the lower or upper plenum, which has large boundary interfaces (the core inlet or outlet planes). More details about it can be found in (Zhang et al., 2020a; Zhang et al., 2020b; Zhang et al., 2020c).

8.3. Coupling of system thermal–hydraulic codes with CFD codes

Based on the experience from SCF/TrioCFD-ICoCo, the system code TRACE was coupled with TrioCFD, based on ICoCo, and the same C++ supervisor. The coupled code's draft is given in Fig. 44.

Different from SCF/TrioCFD-ICoCo, TRACE/TrioCFD-ICoCo adopts the domain-overlapping coupling method. There, like the SALOME-based coupled code TRACE/SCF-ICoCo (under domain-overlapped mode), the simulating regions of TRACE and TrioCFD overlap. Thus

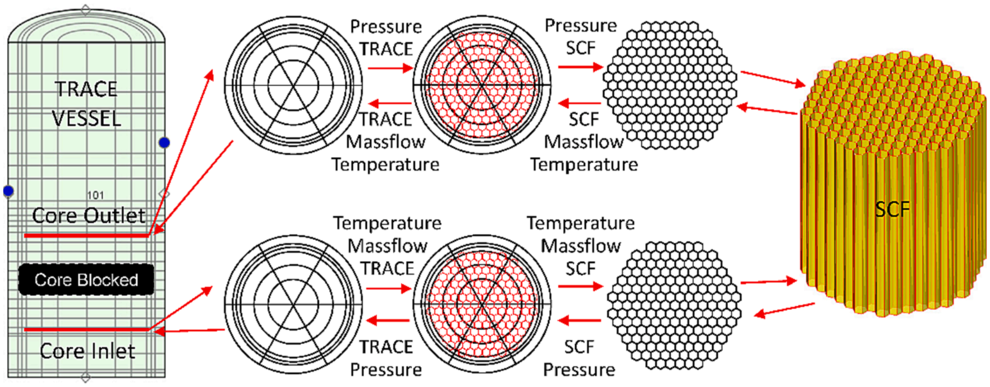


Fig. 39. The thermal–hydraulic coupling strategy of TRACE/SCF-ECI applying the domain-decomposition method. (Zhang and Sanchez-Espinoza, 2019, https://doi.org/10.1016/j.nucengdes.2019.110238).

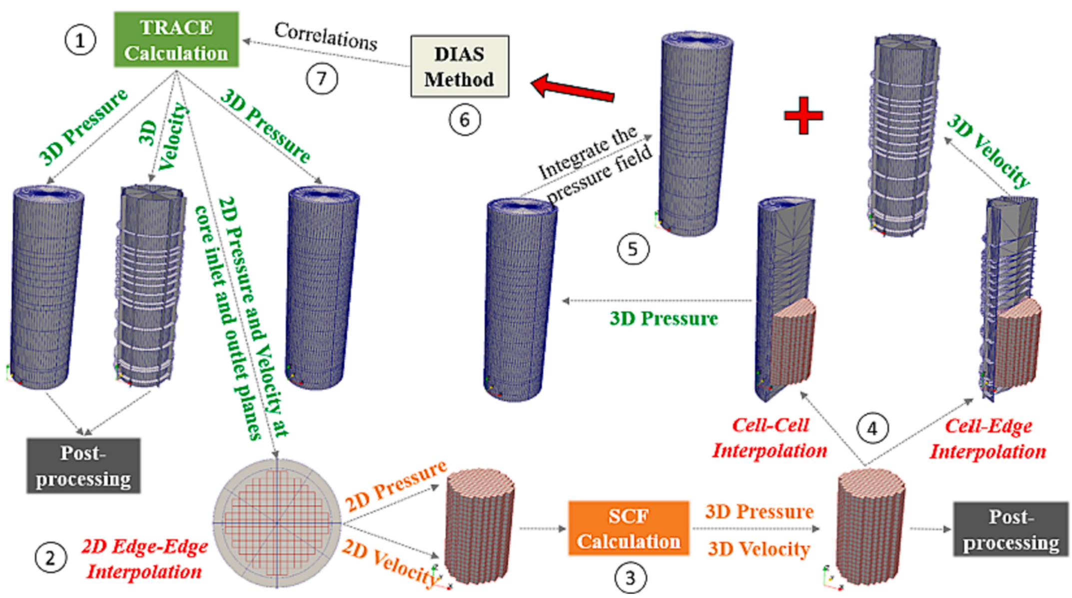


Fig. 40. The hydraulic coupling strategy of TRACE/SCF-ICoCo in SALOME applying the domain-overlapping, explicit mesh, and the DIAS method (Zhang et al., 2021).

Fig. 41. The ICoCo-based coupling code TRACE/SCF-ICoCo under a generic coupling architecture.

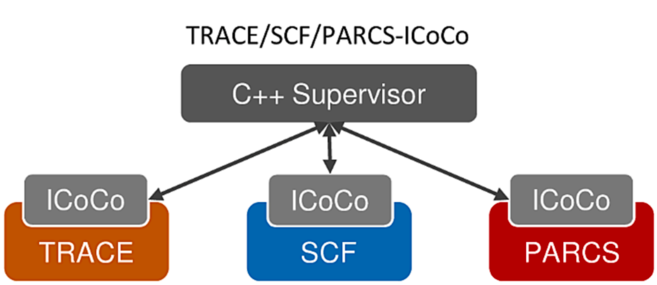


Fig. 42. The ICoCo-based coupling code TRACE/SCF/PARCS-ICoCo under the generic coupling architecture.

the DIAS method is adopted as well. The two codes run in parallel and interact by exchanging 2D and 3D fields every timestep. The field translation between different meshes is handled by the MEDCoupling library. Different from SCF/TrioCFD-ICoCo, the 3D TH fields are transferred from TrioCFD to TRACE in a coupled simulation performed by TRACE/TrioCFD-ICoCo. The data translation is complicated not only because of the dimensionality reduction from vectors to scalars but also because of the transformation from 3D volumic fields to 2D fields on parch grids. As a precondition of correct coupling, the data translation should be tested. In (Zhang et al., 2020a; Zhang et al., 2020b; Zhang et al., 2020c), details of the application of this coupling approach to analyze a VVER-1000 reactor pressure vessel using the coupled code TRACE/TrioCFD-ICoCo are presented and discussed.

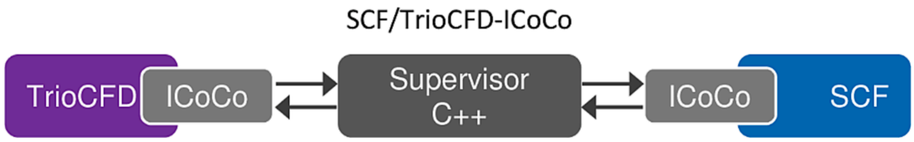


Fig. 43. The ICoCo-based coupling code SCF/TrioCFD-ICoCo.

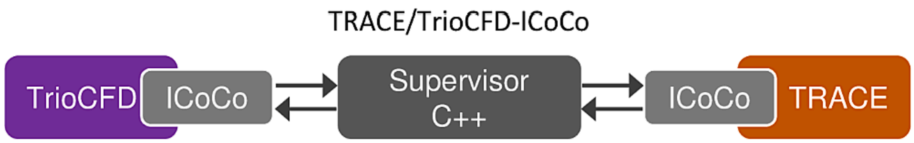


Fig. 44. The ICoCo-based coupling code TRACE/TrioCFD-ICoCo.

It is worth mentioning that the supervisor adopted by TRACE/TrioCFD-ICoCo is the same as the one for SCF/TrioCFD-ICoCo. In this coupling scheme, the open-source CFD code – OpenFOAM is being implemented instead of TrioCFD obtaining the coupled code TRACE/OpenFOAM-ICoCo, see Fig. 45.

This coupled code is now still under development at KIT and is expected to be established and verified shortly. Unlike TRACE/TrioCFD, TRACE/OpenFOAM applies the domain decomposition approach. Within the McSAFER project, the codes are for the multi-scale TH analysis of the KSMR RPV. There, the lower plenum will be modeled by OpenFOAM and the rest will be in the charge of TRACE, as shown in Fig. 46.

Furthermore, to make full use of the generic multi-physics and multi-scale platform, the core neutronics will be simulated by PARCS, which is already equipped with ICoCo. Similar to TRACE/SCF/PARCS-ICoCo shown in Fig. 42, the sketch of TRACE/OpenFOAM/PARCS-ICoCo can be found in Fig. 47. The main difference between the two codes is that PARCS exchanges data with SCF within the former code, while it communicates with TRACE within the latter.

In summary of the above activities, the multi-scale TH development at KIT starts from the coupling of the system code TRACE and sub-channel code SCF based on the ECI interface. Afterward, to make use of the more straightforward coupling interface ICoCo, TRACE, and SCF were equipped with this interface and were coupled together in the SALOME platform. Shortly, the open-source CFD code TrioCFD was coupled to SCF and TRACE independently based on ICoCo. They are supervised by a C++ script which is specially developed for TrioCFD-involved coupling codes. To make the supervisor and coupling architecture more generic and extensible, a new C++ supervisor was developed and the ICoCo interfaces for TRACE, and SCF were refreshed. Within the new system, OpenFOAM was implemented as the CFD solver replacing TrioCFD. In the meantime, efforts were made to implement the neutronic solvers PARCS and Serpent into this system to finalize it as the generic multi-scale multi-physics simulation platform. The overall toolsets that are currently in use are briefly summarized in Fig. 48.

9. KIT experimental facilities and selected code validation

Experimental facilities are very important to improve the understanding of key safety-relevant phenomena and to provide data for the validation of TH and neutronic codes. KIT was running a large number of facilities focused on phenomena related to design basis, e.g. COSMOS-L, COSMOS-H, and severe accidents such as LIVE, MOCKA, QUENCH, etc. Hereafter a short description of the key features of selected KIT facilities and their experimental program will be discussed.

10. The COSMOS-H and –L facilities

The COSMOS-H THs loop, Fig. 49, was completed at the end of 2022 and consists of a high-pressure water loop including a steam generator and an efficient cooling system. The facility was designed for TH experiments under BWR and PWR conditions. It also covers the operating conditions of several light water SMR types. The facility is currently used in the McSAFER project (Sanchez-Espinoza et al., 2021). The objectives of the first experiments in 2023 are to study boiling flows under forced convection up to critical heat flux under typical SMR reactor conditions. The high-pressure loop operates with deionized water and can withstand an operating pressure of up to 17 MPa at temperatures up to 360 °C. The high-pressure loop of COSMOS-H has a thermal power of 1.2 MW and an additional power of up to 600 kW is available to heat the test arrangement. Numerous sensors and control loops are installed to monitor and record water quality, thermodynamic boundary conditions, and the current thermal output of the heating and cooling systems.

The modular test section has a high level of instrumentation and can be flexibly adapted and extended. In its current configuration, the pressure hull of the test section has an inner diameter of approx. 80 mm and a length of approx. 3500 mm. Within this volume, the test section can accommodate various heater configurations ranging from a single rod in an annular gap to a tube bundle, e.g. 4 × 4. Various prototype cladding tube materials such as stainless steel, zircalloy-2, and 4, or, for example, new Accident Tolerant Fuel (ATF) materials can be used in the experimental arrangements. The heating of the experimental setups is done by direct current and initially directly electrically. In the future, indirectly heated rods will also be used. The plant control system enables rapid shutdown of the heating power such that an upcoming boiling crisis can be detected and the heating switched off promptly before the test arrangement is damaged. This is possible for both CHF mechanisms Dryout as well as DNB. Fig. 50 shows the test section prepared for the McSAFER Experiments during the assembly process without thermal insulation and trace heating system. In this configuration, the test section has sensors for pressure, temperature, and heating power as well as two sight glasses with which the boiling flow can be observed using high-speed cameras (Fig. 51).

The high-pressure system COSMOS-H is complemented by the low-

Fig. 45. The ICoCo-based coupling code TRACE/OpenFOAM-ICoCo under the generic coupling architecture.

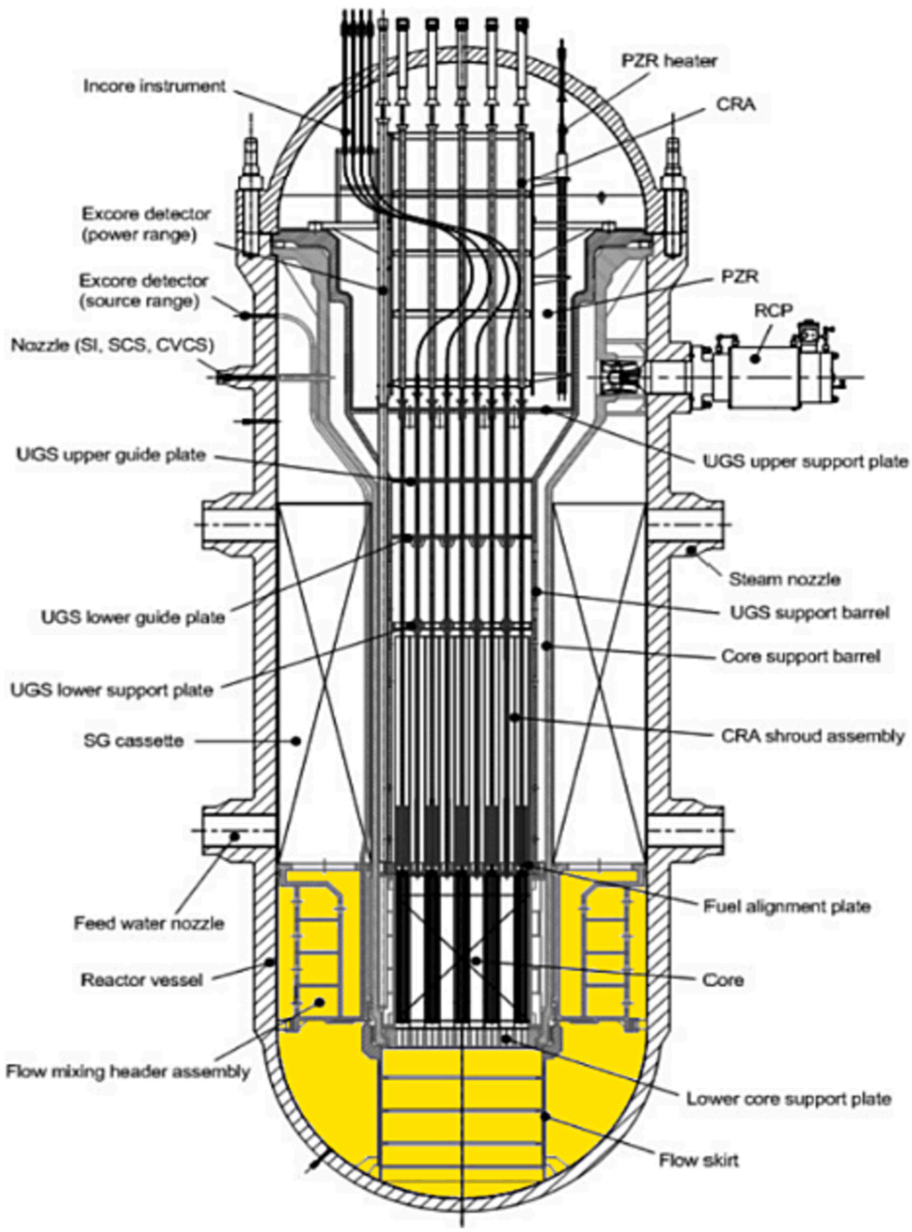


Fig. 46. SMR Reactor Pressure Vessel. CFD domain (in yellow) and TRACE domain (in white).

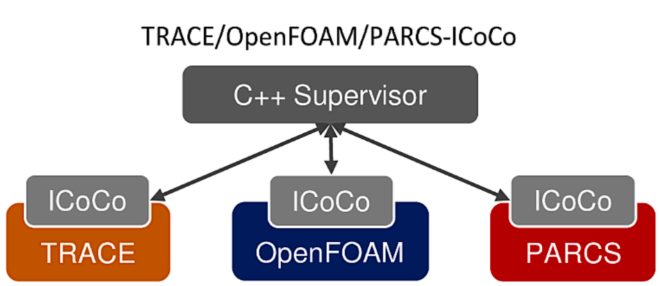


Fig. 47. The ICoCo-based coupling code TRACE/OpenFOAM/PARCS-ICoCo under the generic coupling architecture.

pressure system COSMOS-L, which is much smaller and is operated with a maximum pressure of 6 bar and temperatures up to approx. 220 °C. COSMOS-L was already completed in 2009 and has since been subject to several performance upgrades and modernizations. The test loop, which is also operated using deionized water, currently has a thermal output of approx. 220 kW. Further 70 kW are available for the test section. Mass flows of up to 80 l/min can currently be achieved. Since 2009, the plant has already been used for various thermal–hydraulic investigations on boiling flows up to critical heat flux (Fig. 52).

In (Haas et al., 2018), the behavior of different cladding tube materials with surface structures and their influence on boiling crisis were investigated. It was shown by measurements that there is a significant dependence of the critical heat flux on material and surface modifications. F. Kaiser investigated the boiling behavior up to boiling crisis (DNB type) in systematic parameter variations on a single rod as well as on a small rod bundle both made of Zircalloy-4. In addition to his studies, he also provided extensive data sets for the development and validation of CFD codes in the project NUBEKS. S. Michaelides (Haas et al., 2011), investigated the critical heat flux on a flat heater made of stainless steel (1.4571) concerning IVR-ERVC accident management concepts in the SIMA project. He varied the orientation of the heater from vertical to 45° to horizontal and also considered periodically fluctuating mass flows in his measurement matrix. For this purpose, the loop was equipped with a test section bypass and fast-moving valves to

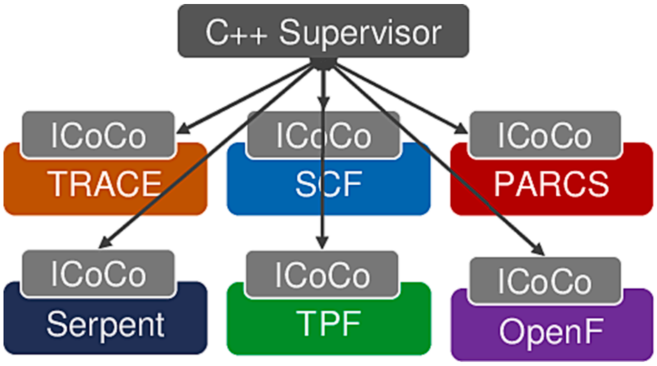
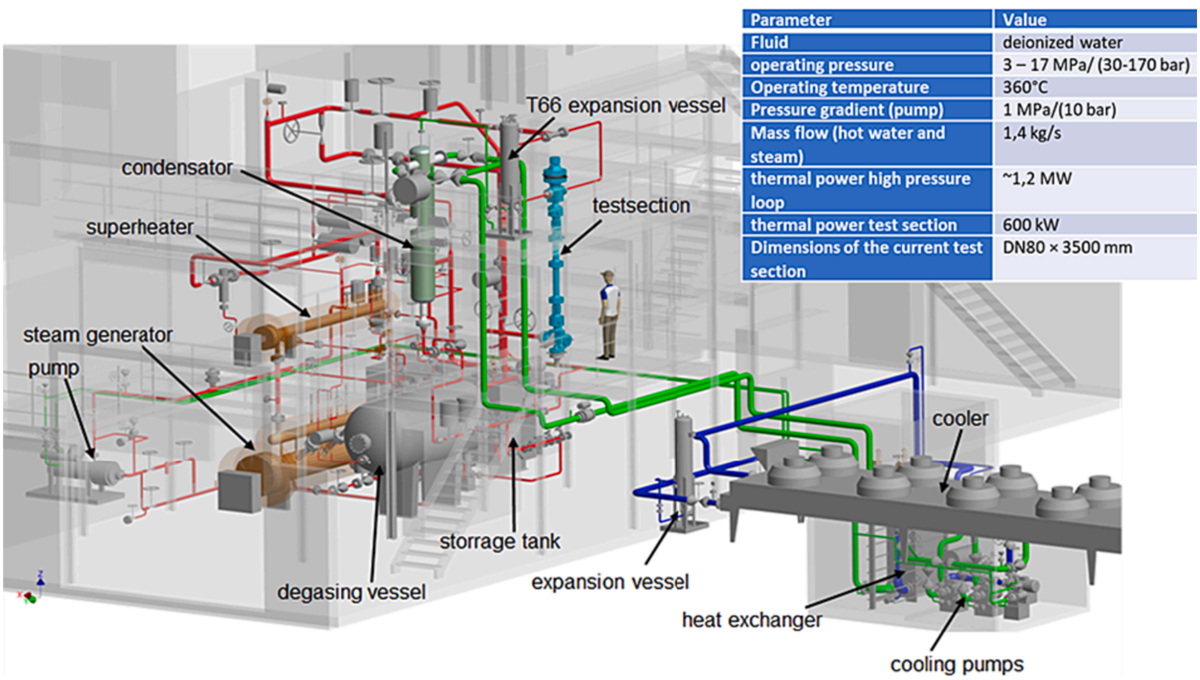


Fig. 48. The generic multi-scale and multi-physics coupling platform that is developed and currently used at KIT.

realize periodic mass flow profiles (period, amplitude, offset). Besides pressure and temperature, mainly different amplitudes and periods of the mass flow were varied, and a considerable influence of the mass flow variations and heater orientation on the critical heat (DNB) was found. The highest critical heat flux achieved was 2.8 MW/m^2 (Frank et al., 2017; Michaelides et al., 2022).

In the current MESA project, various ATF cladding tube materials such as chrome-coated Zircalloy-4 and a FeCrAl alloy are being investigated concerning their boiling behavior and critical heat in comparison with Zircalloy-4. A small tube bundle (length approx. 350 mm) consisting of 5 cladding tubes of each material is used as the test setup. Thereby the central cladding tube is surrounded by 4 others so that the optical accessibility to the central tube is given. The heating power at the central tube is slightly increased with the surrounding tubes, allowing the instrumentation to be concentrated there. The experiments are supported by CFD calculations to minimize measurement uncertainties and evaluate the performance of the different materials as accurately as



Parameter	Value
Fluid	deionized water
operating pressure	3 – 17 MPa/ (30-170 bar)
Operating temperature	360°C
Pressure gradient (pump)	1 MPa/(10 bar)
Mass flow (hot water and steam)	1,4 kg/s
thermal power high pressure loop	~1,2 MW
thermal power test section	600 kW
Dimensions of the current test section	DN80 × 3500 mm

Fig. 49. CAD model and operation parameter of COSMOS-H facility.

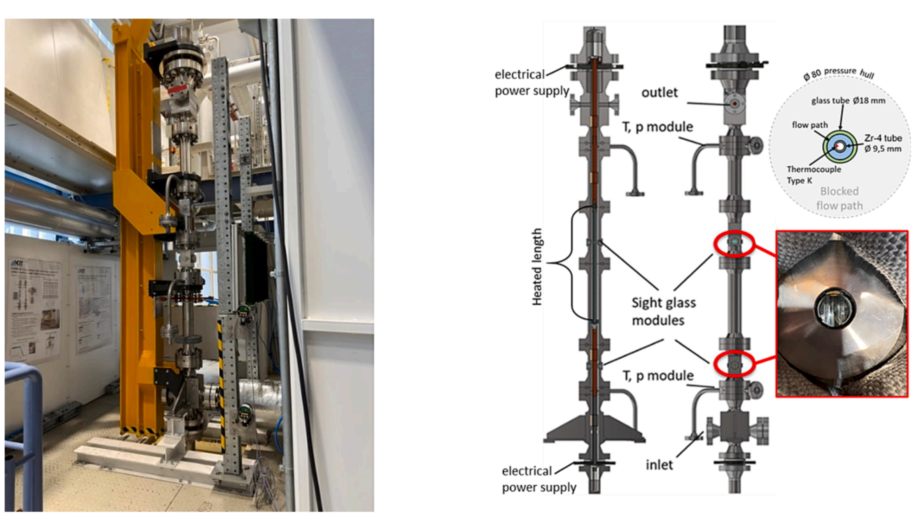


Fig. 50. The test section of the COSMOS-H facility.

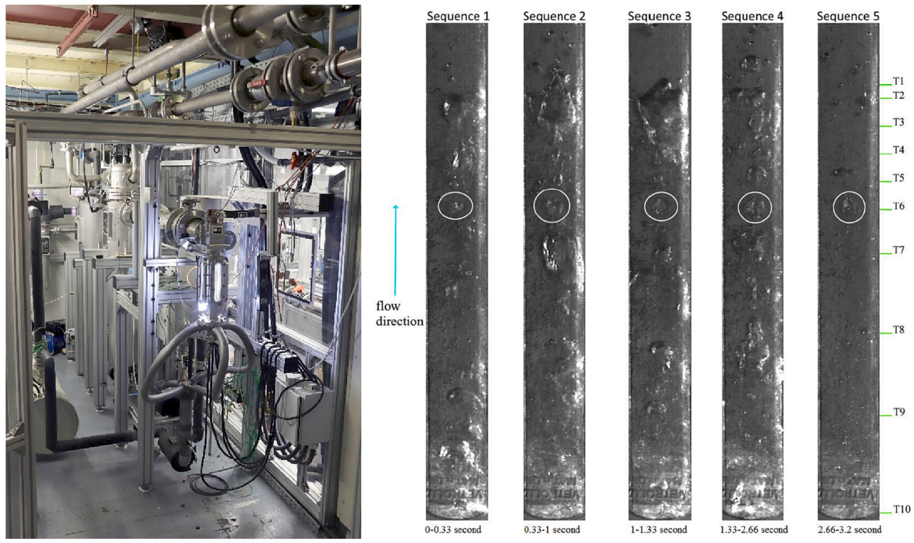


Fig. 51. COSMOS-L Loop and High-Speed Sequence from a DNB event on a flat heater (Michaelides et al., 2022).

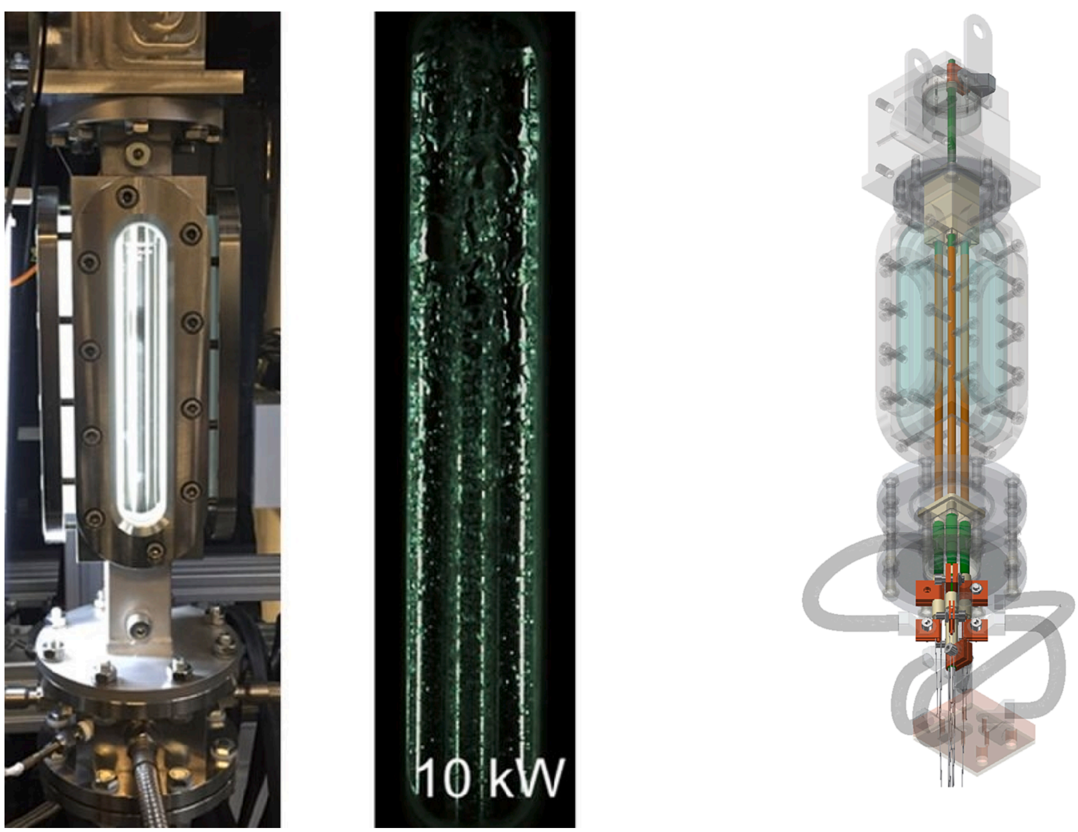


Fig. 52. COSMOS-L test section for investigation of boiling under forced convection in rod Bundles for different ATF materials.

possible.

10.1. The QUENCH facility

The electrical heated out-of-pile facility QUENCH (Steinbrück et al., 2010), Fig. 53, was established in 1997 as the successor of the CORA facility and with similar bundle geometry as the in-pile PHEBUS facility (Haste et al., 2015). The common purpose of the out-of-pile QUENCH facility is to conduct bundle tests on the investigation of fuel cladding-related phenomena during the Design Basis Accidents (DBA, $T < 1200\,^{\circ}C$) and early stage of the Beyond Design Basis Accidents (BDBA or severe accident, $T > 1200\,^{\circ}C$). The QUENCH test facility can be operated in two modes: (a) a forced-convection mode with a flow of about 3 g/s of superheated steam of about 600 °C together with argon, and (b) a boil-off mode with the steam inlet line closed. The system pressure in the test section is usually around 0.2 MPa (max. 0.6 MPa). Quenching can be performed with water or saturated steam from the bottom. The main component is the test bundle that can be of PWR- or BWR-type. The test bundle consists of 21…31 fuel rod simulators, see Fig. 54, with Zr alloy cladding tubes and five grid spacers. The total length of the bundle is about 2.5 m. Heating is electric by tungsten heaters installed in the rod center and surrounded by annular ZrO_2 pellets simulating the UO_2 fuel.

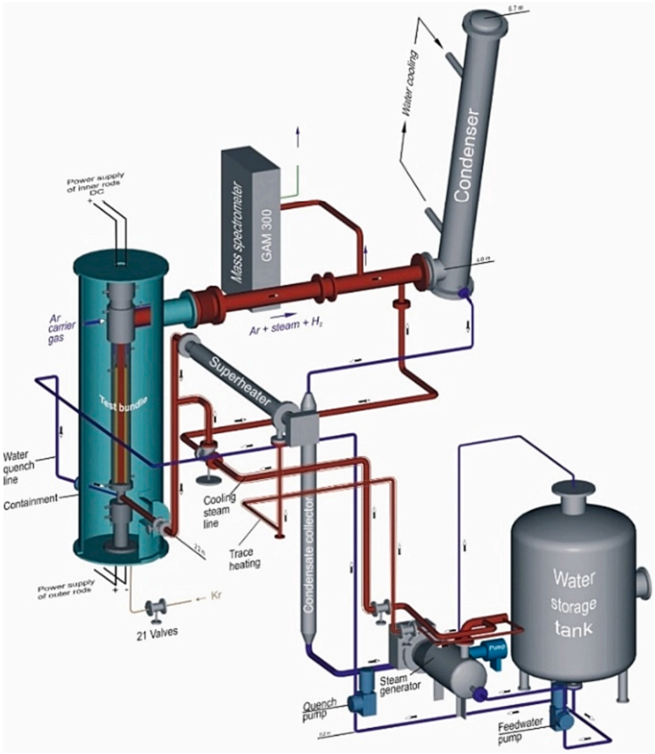


Fig. 53. QUENCH facility.

Electrodes of molybdenum and copper connect the heaters with the DC electric power supply capable of 120…150 kW. Several rods could be unheated and used for instrumentation or as absorber rods, e.g. B_4C or AgInCd to study their influence on core degradation. The test rods could be prefilled up to 14 MPa with Krypton or Helium. The test bundle is surrounded by a 3 mm thick shroud of Zircaloy together with a 37 mm thick ZrO_2 fiber insulation that extends to the upper end of the heated zone and a double-walled cooling jacket of stainless steel/Inconel. Bundle corner rods made of the same material as the rod claddings are either used for thermocouple instrumentation or as probes which can be withdrawn from the bundle anytime during the test to check the amount of oxidation. Regarding DBA research, seven bundle tests with different zirconium alloy-based cladding materials were performed to investigate the influence of the secondary hydriding phenomena on the applicability of the cladding embrittlement criteria (Stuckert et al., 2020). In the BDBA field, twenty high-temperature bundle tests were performed to investigate (Doyle et al., 2023; Stuckert et al., 2021) such effects as a) Temperature escalation due to cladding oxidation and enhanced hydrogen release during reflood, b) Influence of different cladding alloys and cladding coatings on a decrease of hydrogen release, c) Influence of steam starvation and air ingress, d) Formation of eutectics and aerosol release due to influence of neutron absorber rods, e) Debris and melt formation with melt relocation and oxidation, f) Coolability of a blocked bundle.

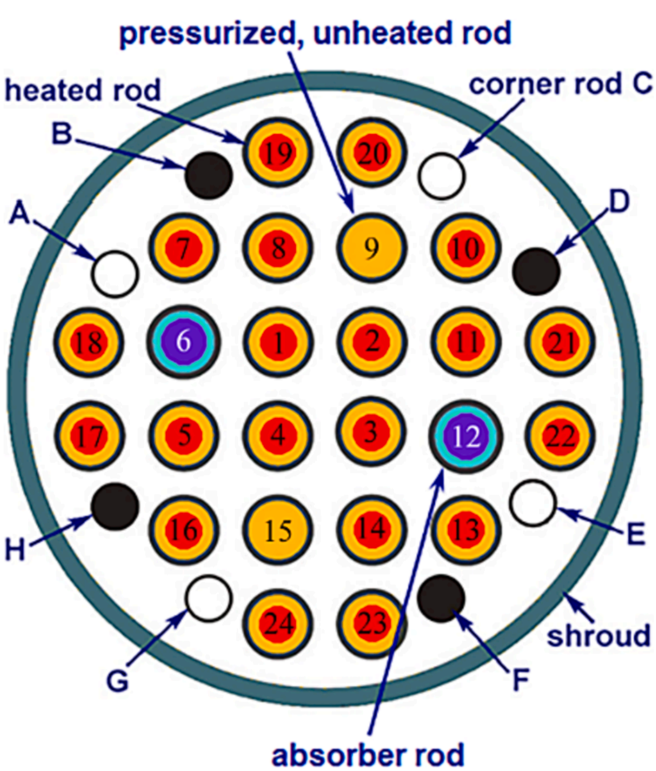


Fig. 54. Cross section of the QUENCH-18 bundle.

In addition, the QUENCH facility can be used to conduct long-term experiments to study the effects that occur in claddings during dry storage of spent fuel assemblies. Currently, the QUENCH facility is an important element for experimental studies on ATF within the framework of OECD and IAEA projects. The experimental data gained during the QUENCH program were used for verification and validation of different computer codes.

10.2. Selected code validation activities using QUENCH-data

The QUENCH tests performed at KIT are permanently part of the validation matrix of the main integral codes worldwide employed, i.e. ASTEC, MELCOR, AC^2/ATHLET-CD. Validation activities of the ASTEC code using the QUENCH experiments have been performed for years at KIT and the outcomes of the most recent analyses are described in the following. The focus of the investigations is the validation of the ASTEC models related to the high-temperature oxidation, melt formation, relocation as well as the chemo-physical eutectic reactions. The reflooding of the overheated rod bundle leads to steam generation and the oxidation of hot metallic surfaces in contact with steam e.g. fuel rod cladding, shroud inner surface. As a result of it, hydrogen is generated not only due to the oxidation of the metallic surfaces but also of the molten material containing metallic. The accurate prediction of these processes is very important to assess the vulnerability of the containment due to the risk of hydrogen combustion, burning, or detonation in a nuclear power plant after a severe accident (Henrie and Postma, 1987). However, the injection of cold water into an overheated core as a SAM measure may result in a rapid increase in the temperature and enhanced oxidation and hydrogen generation (Sehgal, 2012).

10.2.1. ASTEC validation using the QUENCH-12 VVER test data

The main goal of the QUENCH-12 test is to investigate the behavior of an overheated VVER-fuel rod bundle, which is quenched with cold water. Note that in the QUENCH-12 test, the cladding material (E110) used in the VVER NPPs is employed. Since the thermo-physical properties of these cladding differ from the typical materials employed in western PWRs, i.e. Zircalloy, the experiment also aimed at investigating the behavior of such VVER-specific materials by comparison with the outcomes of the QUENCH-6 experiment, where PWR cladding materials were employed. The ASTEC v2.2.0.1 model of the QUENCH-12 test and a detailed analysis of the results are described in (Mercan et al., 2022a; Mercan et al., 2022b). As described in (Stuckert et al., 2009), the test section is loaded by 13 unheated and 18 heated simulator rods arranged in triangles as in VVER reactors, and six corner rods are located to sustain the flow area. The material employed for the cladding and the space grids is Zr-1 %Nb (E110), while the shroud is composed of Zr-2.5 %Nb (E250). Note that the thermo-physical properties and the oxidation laws for E110 and E250 materials are not available in the ASTEC material databank, yet. Having this in mind, Zr-4 has been employed instead. The results show that the ASTEC code can reproduce the experimental results concerning the time-dependent behavior and the oxide scale of the rods. As an example, the calculation results for the oxide scale before the quenching are compared with the experiment in Fig. 55. Concerning the total amount of hydrogen generated, the results in Fig. 56 show some deviations between the ASTEC prediction and the experiment. In particular, the hydrogen generated before and after quenching is overestimated and underestimated by ASTEC, respectively. As extensively discussed in (Mercan et al., 2022b), the employment of Zr-4 instead of E110 and E250 is found the main responsible for this behavior. Nevertheless, the results show that ASTEC can reproduce the main phenomena occurring during the test, in particular the break-away oxidation phenomena of clad structures and the rapid increase of oxidation and hydrogen generation.

10.2.2. ASTEC validation using the QUENCH-20 BWR test data

The QUENCH-20 BWR experiment (Stuckert et al., 2023) was performed to investigate the oxidation, hydrogen generation, melt formation, and oxidation during the reflooding of a test bundle representing a quarter of an SVEA-96 Optima-2 fuel assembly. An ASTEC v2.2.b model of the QUENCH-20 test has been developed at KIT. A detailed description of the model and the validation against the experiment is provided in (Murat et al., 2020). The bundle is composed of 24 electrical heated rods, 5 Inconel X750 spacer grids, half of a canister, half of an absorber blade representative of the B4C + SS and SS rods, and the shroud. The test consists of a pre-oxidation phase (until 14,400 s), a transient phase (up to 15,890 s), and a quenched phase, where water is injected into the bundle with a flow rate of 50 kg/s. The test ends at 16,890 s. The results show that the ASTEC code can reproduce the main phenomena occurring during the transient. In particular, the time-dependent behavior of the heated rod temperature calculated by ASTEC is in quite good agreement with the experiment. The results concerning the total amount of hydrogen generated during the test as well as on the amount of hydrogen produced by the oxidation of the B_4C blades are shown in Fig. 57. It may be observed that the ASTEC results concerning the total amount of hydrogen produced well reproduce the experiment concerning both the time-dependent behavior and the mass. In particular, at the end of the transient, ASTEC predicts 53.4 g of hydrogen produced, which is in good agreement with the experiment (57.4 g). Furthermore, the mass of hydrogen due to the oxidation of the B_4C predicted by ASTEC (9.48 g) is in very good agreement with the experimental data (10 g).

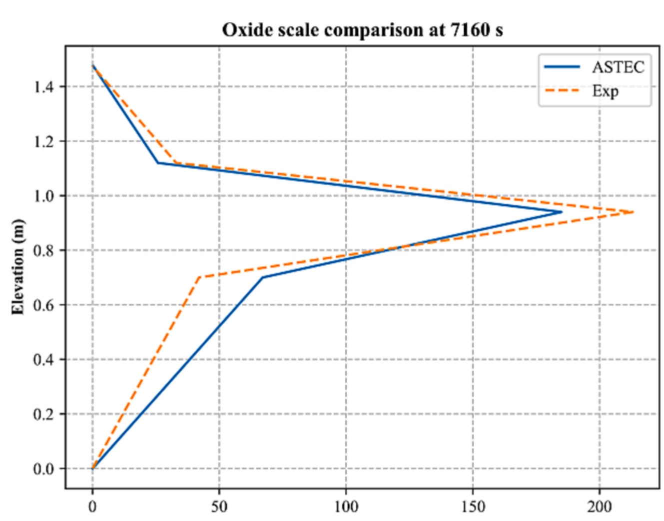


Fig. 55. Measured versus predicted (ASTEC) oxide scale results for corner rods before quenching.

10.2.3. ASTEC validation using the QUENCH-19 ATF test data

The ATF cladding materials have the potential to improve the safety performance of large and integral LWRs during normal and transient operations as well as during hypothetical severe accident scenarios.

Compared with the Zr-based cladding currently employed in LWRs, one of the main goals of the use of ATF materials is the strong reduction of the kinetics of steam oxidation leading to slower heating and then a longer period before the temperatures reach the melting point. Having this in mind, large efforts are going on worldwide, and in particular at KIT, to investigate the behavior of different ATF cladding materials in DBA and BDBA conditions. In parallel, efforts are also going on to extend the modeling capabilities of the integral codes, mainly developed for reactors employing Zr-based cladding, to enable the safety assessment of the innovative reactor concepts employing such materials, i.e. SMRs (Hollands et al., 2022). Having this in mind, research activities are going on at KIT to validate the ASTEC code against the QUENCH test devoted to the investigation of ATF materials. The QUENCH-19 test was performed in 2008 to investigate the behavior of FeCrAl as a cladding material in a test bundle composed of 24 heated rods and 8 corner rods (Stuckert et al., 2022). The test conduct as well as the bundle arrangement is similar to the QUENCH-15 test, where Zirlo cladding was employed. To develop and extend the ATF-related modeling capabilities of the ASTEC code, a model (v2.2.b) of the QUENCH-19 test has been developed at KIT (Gabrielli et al., 2021; Hollands et al., 2022; Gabrielli and Sanchez-Espinoza, 2022). As described in (Hollands et al., 2022; Gabrielli and Sanchez-Espinoza, 2022), the FeCrAl oxidation model based on (Kim et al., 2022) has been first employed. The preliminary ASTEC results concerning the hydrogen generated during the QUENCH-19 test are compared with the experimental data in (Gabrielli and Sanchez-Espinoza, 2022). The ASTEC results, Fig. 58, show an acceptable agreement with the experiment concerning the time-dependent behavior of the hydrogen produced as well as on the total amount, while deviations can be observed in the kinetics of the escalation.

Despite the reasonable results, it is worth mentioning that the extension of the ATF-related modeling in the ASTEC code is going on. Many efforts have been spent at KIT mainly on the development of an ATF-dedicated material databank, which of course is directly related to the advancements in the experiments.

11. Summary & outlook

The paper describes the experimental and analytical research activities for the safety assessment of LWR and water-cooled SMRs of different designs including the radiological source term prediction and its dispersion around the site. The emphasis is put on the KIT tests facilities and codes being developed and validated at KIT as well as its application.

The KIT developments are focus on the core comprasing both neutronics (PARAFISH code) and thermal hydraulics (SCF and TPF codes), used for the analysis of the core behavior under nominal and transient conditions. These tools are intended to improve the core analysis (neutronic and THs), by using subchannel codes and neutron transport solver instead of 1D system TH codes and diffusion codes. Moreover, the tools are being validated using relevant data for LWR such as PWR, BWR, VVER, and research reactors with MTR-fuel type. The neutronic code is being validated in the frame of international benchmarks of the OECD. An important motivation for the development of PARFISH and TPF is the simulation of the reactor physics behavior of SMR-cores under static and transient conditions not only at nodal but also at pin/subchannel level. For the mutliphysics coupling, the ICoCo interfacend the MEDcoupling libraries are used, which are modular and very flexible.

In addition, KIT is engaged in the development of high-fidelity coupled tools aiming to perform very detailed core analysis, i.e. at the pin/subchannel level taking into account the local feedback between neutronics, THs, and thermo-mechanics thanks to the versatility, robustness, and the prediction capability of tools such as Serpent2, SCF,

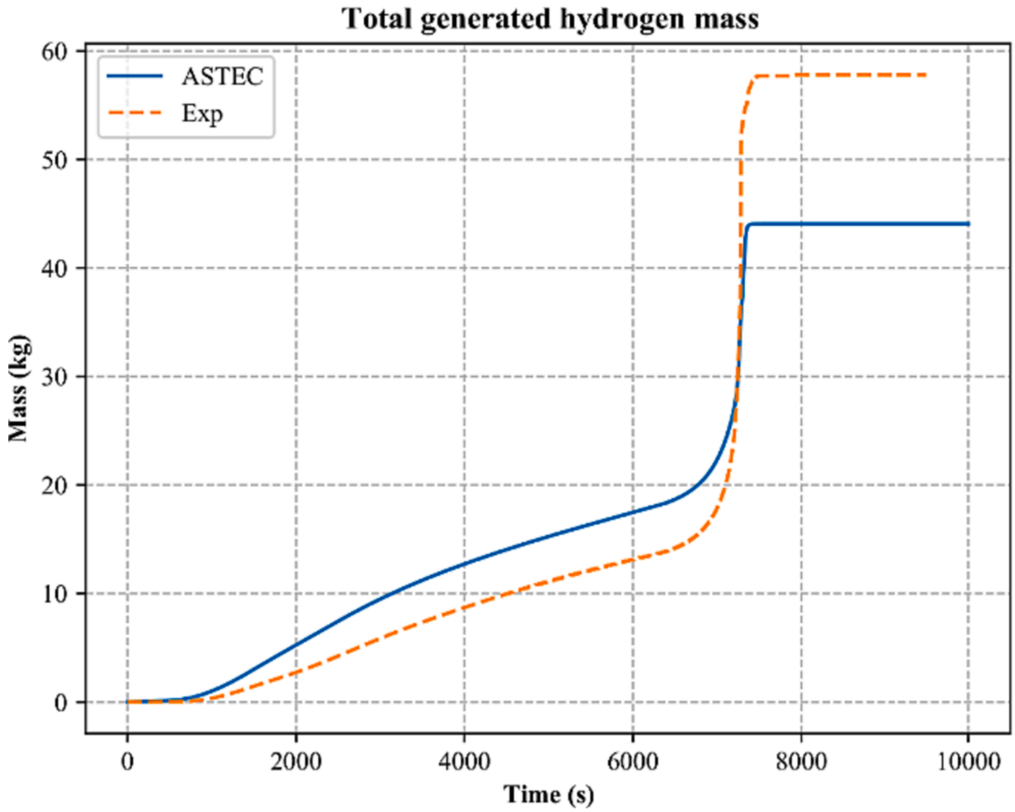


Fig. 56. Measured versus predicted (ASTEC) hydrogen generation.

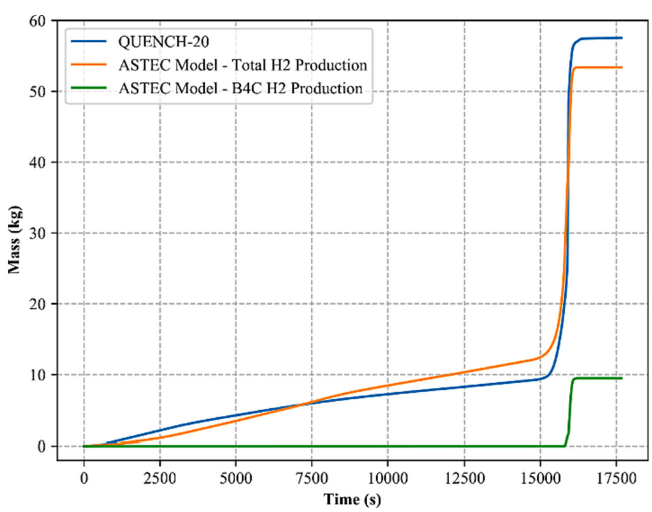


Fig. 57. Cumulative hydrogen generation of QUENCH-20 test and ASTEC model due to oxidation.

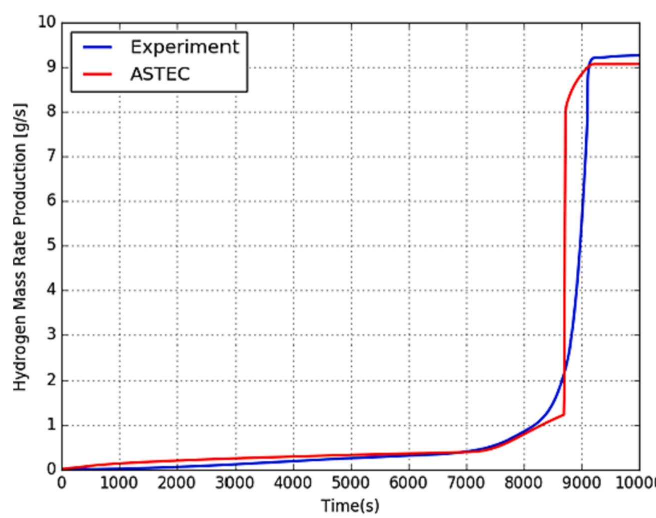


Fig. 58. Measured versus predicted (ASTEC) hydrogen generation in the QUENCH-19 test.

and TU. These tools paved the way for unique whole core pin/sub-channel level simulations using large computer clusters of KIT. First steps for the validation of such tools were undertaken e.g. the dynamic capability of Serpent2/SCF using unique data of the SPERT REA tests as well as data NPP such as the Pre-Konvoi PWR and of the Temelin plant. The promising results obtained by the validation was a pre-conditions to apply these tools for the simulation of transient of SMR and research reactors with MTR-cores. Novel results were obtained and published.

Another pillar of the KIT developments is the multi-scale/-physics code developments based on the ICoCo-approach, where system TH codes are coupled with subchannel and CFD to increase the prediction accuracy of 3D TH phenomena inside the core and RPV of LWR of generation I, II, and III. At present, the focus of such developments is the enhanced analysis of water-cooled SMR with integrated RPV, where multi-dimensional phenomena play a key role and for which the 1D TH codes are no longer appropriate.

To understand new safety relevant phenomena in LWR with new fuel such as the ATF and in water-cooled SMRs, KIT is operating two test facilities and diverse single effect test devices with focus on both design basis and severe accidents. In the past, the majority of tests at the QUENCH facility were devoted to investigating the behavior of rod bundles of PWR, VVER, and BWR under the early phase of severe accidents. The COSMOS-L/-H facility is devoted to the study of fundamental TH phenomena of safety relevance in LWR belonging to the design basis accidents.

Recent investigations in the QUENCH facility are devoted to experimental investigations of ATF-fuel in the frame of international OECD/NEA activities while the current COSMOS-H experimental program is devoted to studying safety-relevant phenomena in the core of water-cooled SMR in the frame of the EU McSAFER project.

Finally, KIT has also developed own tools for the quantification of the radiological consequence (JRODOS) after hypothetical severe accidents with large release of radioactive material and tools for the quantification of the sensitivity and uncertainty (KATUSA) of any kind of numerical tools in use at KIT.

It can be stated that KIT has all key simulation tools needed for both safety assessment and estimation of the radiological risk including its dispersion after hypothetical severe accidents occurring somewhere I in the world, namely: simulation tools for neutronics, thermal hydraulics, severe accident phenomena, and radiological dispersion.

Future safety-related research activities at KIT are focused on areas of high relevance for the safety of all reactor types under operation around Germany and worldwide, especially on SMR, and on ATF-fuel relevant for all reactor types. Important topics to be explored in the future are artificial intelligence, big data, and the optimization of parallelized numerical tools to take profit of the huge computer power available at KIT e.g. in the HPC HOREKA. The final goals is to improve the prediction capacity and accuracy of the numerical tools for design optimization and safety assessment of nuclear reactors of different type. Hereafter is a list of selected topics of interest is given:

- Experimental programs at QUENCH and COSMOS facilities related to design basis and severe accident for both LWR and SMR considering the core loading with ATF fuel;
- Code developments and validation:
- ▪ Improvements of the TWOFORFLOW for SMRs, parallelization for pin/subchannel level simulations, coupling with different neutronic solvers (Monte Carlo and transport);
- ▪ Extension of PARAFISH solver with time-dependent capability, coupling with TH solvers, validation, parallelization based on domain decomposition, application to SMR-cores;
- ▪ Extend validation of high-fidelity multi-physics/-scale numerical tools for the safety of LWR and application to SMRs, innovative reactors, and research reactors;
- Extension of severe accident codes for the analysis of water-cooled SMR, model development to describe the behavior of ATF under accidental conditions in close cooperation with partners;
- Artificial intelligence and uncertainty quantification methods in nuclear engineering (EU ASSASS project);
- Potential application of high-fidelity tools for research reactors, innovative SMR, etc.
- Involvement and education and training at KIT and worldwide to disseminate the accumulated knowhow and the use of the KIT-tools and results of experimental and analytical investigations.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The authors do not have permission to share data.

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