KIT Numerical Simulation Tools for the Transient Analysis of Water-Cooled Small Modular Reactors

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ABSTRACT

Small Modular Reactors (SMR) gained increased interest worldwide including in Europe. Two new designs (NUWARD, LDR-50) are being developed in France and Finland. Designs like NuScale and BWR-X-300 are being discussed to be built in Poland, Bulgaria, Sweden, etc. Other SMRs such as CAREM, ACP100, and RITM-200N are under construction. Appropriate numerical tools are needed for the safety evaluation. In the EU, different projects such as ELSMOR, TANDEM, McSAFER, etc. are focused on the licensing, integration in the energy mix, thermal-hydraulics, experiments for thermal -hydraulic phenomena (cross-flow, performance of helical HX, CHF), and safety evaluation methods. In the frame of the McSAFER-project and of the BMBF Innovation-Pool for SMR-safety, KIT is developing new core physics codes (neutron transport, 3D thermal hydraulics) as well as multi-physics and -scale methods. This paper will present and discuss the status of the code development, their application to SMRs and the perspectives. Selected results of different studies performed at KIT will be described and discussed. The goal of these developments is two-fold: improve the neutronic and thermal-hydraulic simulation of SMR-cores by developing transport and 3D thermal-hydraulics methods at pin/subchannel level.

Keywords: Water-cooled SMR, TWOPORFLOW, SUBCHANFLOW, PARCS, PARAFISH, Serpent2, Multiphysics, transients

1. INTRODUCTION

The deployment of Small Modular Reactors (SMR), and in special water-cooled SMRs have experienced a considerable progress [1]. Many EU countries are discussing the construction of SMRs within the next decade e.g., Poland, Sweden, France, Finland, Czech Republic. European designs such as the NUWARD [2] and the LDR-50 [3] are in the advanced design phase. Both designs rely on boron-free cores built of shorter standard Fuel Assemblies (FA) of type FA 17x17-25. NuScale [4] and SMART [5] use the same FA-design but they consider boron in the coolant. In general, SMRs are designed for electricity generation, water desalination, industrial heat production, hydrogen production, etc. The BWR-X-300 is going to be built in Canada, Poland, and Sweden [6]. It works without pumps based on natural convection as the larger ESBWR unit [7]. The CAREM [8], ACP-100 [9] and the RITM-200N [10] are under construction in Argentina, China, and Russia. In Canada, the BWR-X-300 was selected for new-build and demonstration by 2028 [11]. In the EU, different projects such as ELSMOR [12], McSAFER [13], are focused on the licensing, experiments for thermal-hydraulic phenomena (cross-flow, performance of helical heat exchanger, CHF), and safety evaluation methods for the core and plant behavior. KIT is involved in McSAFER and German SMR-projects, where the

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focus is the development of new core physics codes (neutron transport, 3D thermal hydraulics) as well as multi-physics and -scale methods for the analysis of core and plant transients. In this paper, the computer codes under development and verification will be described first. Then selected applications of the stand-alone codes to analyze SMR-cores are presented to show their simulation capability. Finally, examples of the application of multi-physics coupled codes developed at KIT and will be presented and discussed. After the conclusions, an outlook about further development directions will be given.

2. TOOLS FOR IMPROVED CORE ANALYSIS

In this chapter, the challenges of the thermal hydraulic phenomena in water-cooled SMR and of the safety-related tools under development at KIT will be presented.

2.1. Core thermal hydraulics challenges

The constructive, operational, and design peculiarities of the water-cooled SMRs being constructed and developed represent new challenges for the thermal hydraulic codes [14]. First of all, the core height is about half as the one of large Pressurized Water Reactors (PWR), and the number of FAs in the core is between 30 to 200. The FA-design can be square or hexagonal (CAREM, RITM-200). The heat removal during normal operation is based on natural circulation (e.g., NuScale, CAREM) or forced convection (e.g., SMART, NUWARD, ACP100). In some designs, boron is considered in the primary coolant (e.g., NuScale, ACP100) while other designs are operated without boron (e.g., CAREM, SMART, NUWARD). The integrated Reactor Pressure Vessel (RPV) is hosting many big components as canned pumps, heat exchangers (Helical coiled, plate-type, etc.) and pressurizer (PZR). These constructive peculiarities disturb the flow inside the RPV, resulting in a 3D mixed convection. Hence, new experiments are needed to study safety-relevant phenomena like CHF, cross-flow, transition from forced to natural circulation and vice-versa under normal and accidental of SMRs. In McSAFER, experiments for water-cooled SMRs are performed at three facilities (MOTEL, HWAT, and COSMOS-H), which will provide data for code validation. KIT is developing 3D thermal hydraulic codes for subchannel level analysis of SMR-cores, which can be used stand-alone or coupled with different reactor dynamic codes for safety-related analysis. In the next subchapters, the key features of SUBCHANFLOW (SCF) and TWOPORFLOW (TPF) will be described.

2.1.1. The subchannel code SUBCHANFLOW (SCF)

SCF is a fast-running, flexible code for rectangular, hexagonal, and plate fuel bundles and full core analysis. The physical models describe the main physical phenomena occurring in sub-channel flow under steady-state or transient conditions. These problems are solved iteratively with a fully implicit solver, where the flow is restricted to upward direction including lateral exchange. Another solver based on the semi-implicit SOLA method [15] describes flow with low flow rates, downward, and buoyancy-driven flow. The heat transport from the fuel rods to the fluid is based on a cylindrical one- dimensional radial heat conduction model including the gap conductance between the fuel pellets and the cladding. In SCF, the total flow rate or a channel-dependent flow rate can be used as boundary condition at core inlet. There, the flow can be distributed automatically to the parallel channels depending on the friction at the bundle inlet. Different empirical correlations for pressure drop, heat transfer coefficient, void generation, etc., were implemented for Light Water Reactors (LWR) and Material Testing Reactors (MTR) [16]. In SCF, 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. Specific models of SCF were validated using experimental data from PSBT and BFBT tests [17].

2.1.2. The porous-media two-phase code TWOPORFLOW (TPF)

TPF is being developed at KIT as a two-fluid code for 3D Cartesian geometry according to the porous-media approach. It solves the time-dependent system of six conservation equations describing two-phase flow including boiling and heat transfer on a heated structure and interface [18]. The porous medium approach used in TPF is used to model the geometrical details not explicitly represented in the 3D 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 3D-cell that contains both fluid and solid phases. The two-fluid model uses separate partial differential equations for the conservation of mass, momentum, and energy for each fluid phase. A large number of empirical correlations are implemented to describe the exchange of mass, momentum, and energy between the phases and to close the system of equations. The friction and heat transfer on the wall of the solid structures is also predicted by respective correlations. The system of equations is solved by a semi-implicit technique for a staggered spatial mesh, where the momentum terms are predicted at the cell boundaries and all scalar quantities at the center of the cells. It is important to highlight that apart from the porous media approach, the heat transfer between a fuel rod and the coolant is based on a cylindrical 1D radial heat conduction model including the gap heat transfer. TPF is very flexible to simulate a reactor core depending of the required spatial resolution of the analyst. For example, several rods in one computational cell can be represented by an average rod. Hence, a FA can be represented radially by a cell, or subdivided in 4, 8, or more cells. Hence, it is also feasible to perform a pin/subchannel level simulation of a SMR-core, where in a radial cell, the pin and the coolant are considered. 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 are implemented and validated [18], [19].

2.2. Core neutronics challenges

The small and compact design of water-cooled SMRs is characterized by a radially very heterogeneous core loadings, massive use of burnable poisons (especially for the boron-free cores), a heavy reflector, different fuel assembly designs with different enrichment and number of control rods with different absorber materials (radially and axially). These core features are challenging the current industry-like diffusion codes. To overcome these limitations, the development of neutron transport solvers using higher-order solutions and a multigroup approach is needed. Nodal diffusion solver coupled to 1D thermal hydraulics does not allow the direct prediction of safety parameter; they rely on pin power reconstruction and the use of hot channel factors. In the meantime, the coupling of subchannel codes with deterministic transport [20] or Monte Carlo codes [21] paves the way for direct prediction of safety parameters for SMR-cores.

2.2.1. The neutron transport code PARAFISH

PARAFISH is a deterministic neutron transport code based on the even parity approach [22] that performs core simulations in 2D/3D Cartesian geometries under stationary conditions using the multi-group approximation for the energy, the non-conforming finite elements for the space and spherical harmonics expansion (PN) for the angular discretization. The advantage of the PN approximation is that the equations are invariant under rotation; therefore, it does not suffer ray effects (non-physical numerical behavior). Currently, the code interacts with high-quality open-source libraries such as PETSc [23] for solving large sparse matrices and SLEPc [24] for computing large eigenvalue problems. PARAFISH has been verified successfully with classical benchmarks [25], [26]. Internal evaluations of the PN method concluded that it requires enormous RAM-capacity when 3D problems are solved due to a large number of unknown equations. Hence, an extension of the PN-solver to analyze 3D transients is not affordable. Based on the review of the international trends, the Simplified PN solver (SPN) [27] was identified as promising option for PARAFISH full-core static and transient analysis at pin-level. At present, the implementation of the steady-state SPN-solver is ongoing.

2.3. Multiphysics coupling for improved core analysis

Selected multi-physics coupling approaches implemented at KIT using mainly in-house codes for the improved analysis of the SMR-core behavior under normal and off-normal conditions are briefly described.

2.3.1. ICoCo-based coupling of PARCS/SCF

KIT has been continuously working on the coupling of SCF and the neutronic codes e.g., DYN3D [20], PARCS [28] for couples of years. Now PARCS and SCF are coupled using modular and flexible ICoCo-interface. The coupling principle is given in Figure 1. There, PARCS and SCF act as two clients and their execution are coordinated by a C++ supervisor via the ICoCo interface.

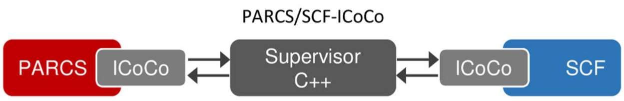

Figure 1. Diagram of the IcoCo-based coupling code PARCS/SCF [29].

This is a server-client system with the parallel capability based on MPI. The codes can iterate explicitly or semi-implicitly and their communicating data are translated by the MEDCoupling library [30] which is part of the open-source SALOME platform. This coupled code is intentionally developed for the SMR safety analysis on the assembly level. The same method was used to couple PARCS and SCF at pin-level [31] for direct prediction of safety parameters.

2.3.2. ICoCo-based coupling of PARCS/TPF

PARCS and TWOPORFLOW are coupled based on a two-way external coupling scheme, where the data exchange is performed using ICoCo, Figure 2. The data is transferred applying a domain-overlapping node-wise feedback mechanism in each iteration. In this scheme, PARCS provides a detailed 3D power distribution to TWOPORFLOW. Latter computes the thermal-hydraulic parameters, e.g., fuel temperature, coolant temperature, and coolant density to be transferred PARCS [32].

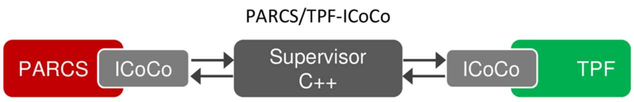

Figure 2. Diagram of the ICoCo-based coupling code PARCS/TPF [29].

2.3.3. Internal coupling of Serpent2/SCF

The Monte Carlo code Serpent2 was coupled with SCF based on internal coupling master-slave approach [33], where SCF is compiled as a shared library and included in Serepent2. Additional coupling routines were written to control the coupled calculation sequence e.g., initialization, transfer of TH-fields, relaxation, convergence, and finalization. The coupled code is very versatile, allowing the simulation of different problems such as steady-state, burnup, and transient dynamic simulations [34]. This tool is extensively used within the McSAFER-project for the analysis of SMR-cores.

3. SELECTED NEUTRON PHYSICAL ANALYSIS OF SMR-CORES

In this chapter, selected results of ongoing investigations of SMR-cores in-house stand-alone thermal-hydraulics and neutronics codes are presented and discussed.

3.1. TWOPORFLOW (TPF) analysis of the NuScale core at subchannel /pin level

A Python-based pre-processor was developed to generate both FA/channel and pin/subchannel level input data as required by TPF. It needs few geometrical data of the SMR-core e.g., fuel assembly type and pin/guide tube arrangement, pin pitch, etc. Then, a node- and pin-wise static simulation of the NuScale core was done with TPF for full power conditions. The node-wise core model consisted of 1225 3D cells while the pin-wise core model has 354025 3D cells considering 25 axial nodes of a 2D grid of 7x7 in case of the node-wise and 119×119 in the pin-wise solution approach. In both simulations, a cosine-shaped axial power profile was assumed. For the radial power per FA, the node-wise power fraction was transferred to the corresponding fuel rod in the pin-wise case.

Table 1. NuScale results comparison for node-wise and pin-wise calculations.

Parameter	Node-wise	pin-wise
Core heat-up (K)	55	55
Core pressure drop (kPa)	10	10
Maximal fuel temperature (K)	919.01	933.86
Maximal cladding temperature (K)	880.44	880.70

It can be observed that the global results are similar while the local parameters differ from each other. The pin-wise simulation predicts a higher maximal fuel cladding temperature compared to the one of the node-wise. It is worth to mention that the run time needed for the pin-wise simulation of the NuScale core by TPF is 1.26 h compared to the 12 sec of the node-wise simulation showing that TPF is running fast. The successful simulation of the NuScale core at subchannel/pin level is very promising since it paves the way for coupled simulations of TPF with a transport or Monte Carlo solvers to predict local safety parameters.

3.2. PARAFISH steady state analysis of NuScale core

A static analysis of the NuScale core was performed with PARAFISH for verification purposes. The core specifications were taken from [35]. CASMO5 was used to generate a set of homogeneous cross-sections. The analysis was conducted under steady-state condition, at the beginning of the cycle (BOC) state, and with all rods out (ARO). The results obtained using a P_7 approximation with a set of 4 energy groups were compared to the ones of Serpent2 reference [35]. The predicted k_{eff} (1.03170) differs from the one (1.02768) of Serpent2 by 391 pcm. Regarding the Assembly power, Figure 3 illustrates the error and distribution. As can be appreciated, the differences are in acceptable agreement, except for the assembly with gadolinia (2.36%). For improving the results, modeling the core with a higher resolution at the pin level should reduce the differences.

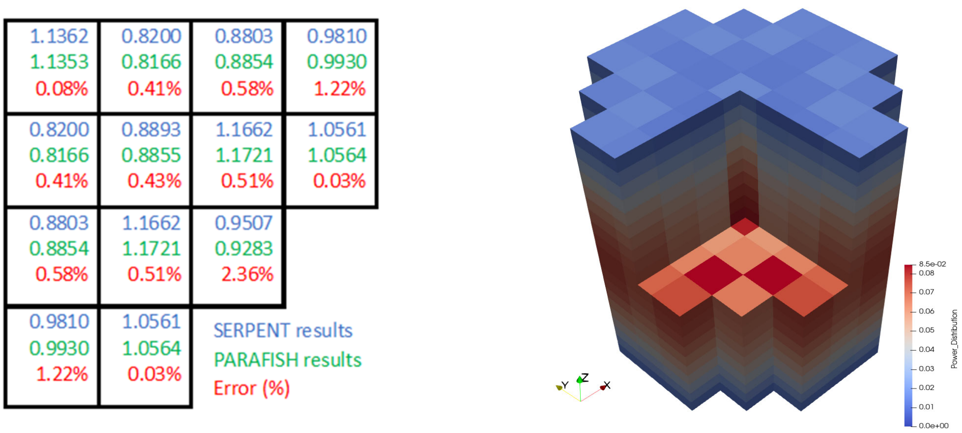

Figure 3. Analysis of a NuScale-like core with PARAFISH; (left): Overall Assembly Power Error, (right): 3D Power Assembly Distribution.

4. SELECTED MULTIPHYSICS ANALYSIS OF SMR-CORES

In this chapter, results of transient analysis of selected SMR-cores using multi-physics coupled codes are presented and discussed.

4.1. NuScale REA Analysis with PARCS/TPF at FA/channel level

A Rod Ejection Accident for NuScale was analyzed with PARCS/TPF/ICoCo at FA/channel according to the scenario described in [36]. The ejection of a single control-rod assembly (CRA) at 75% of nominal power is considered. The transient starts with the CRA-ejection at constant speed within 0.1 sec inserting 0.23$. Then, the transient evolves until 2 sec determined by the neutronic-thermal hydraulic feedbacks. The remaining CRA are fully inserted at constant speed within one second, except for the ejected CRA and a neighboring CRA. The transient ends after 4 sec. The PARCS/TPF simulation predicted a slow power increase of 30%, reaching its maximum value at 0.66 sec. Figure 4 shows some of the safety parameters demonstrating the core coolability during the REA. The peak fuel enthalpy reaches a maximum value of 39.66 cal/g, while the fuel enthalpy change is about 2.5 cal/g. These values meet the acceptance criteria of the US-NRC [37]. Figure 5 shows the 3D power distribution at the time of the highest total power during the transient evolution.

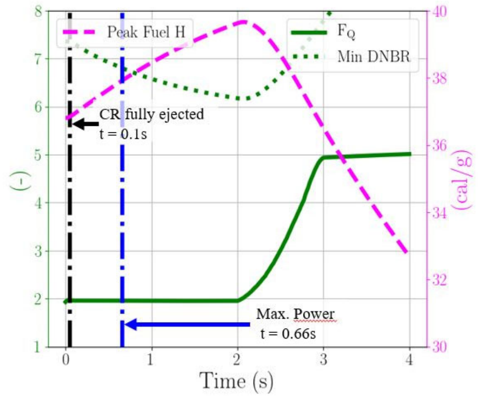

Figure 4. NuScale safety parameters followed during the REA.

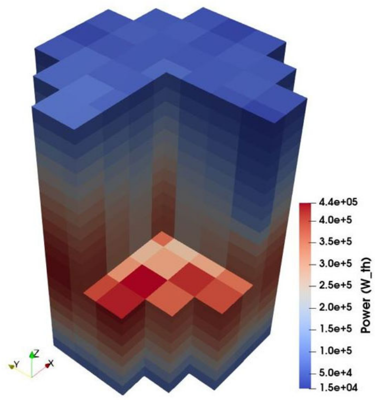

Figure 5. NuScale 3D power distribution at the time of maximum power.

4.2. KSMR REA analysis with PARCS/SCF at pin /subchannel level

PARCS/SCF diffusion solver was used to analyze a REA of the KSMR-core. It consists of 57 FA of 6 types and 2 absorber types with radial and axial heterogeneity [31]. The control rod configuration is depicted in Figure 6.

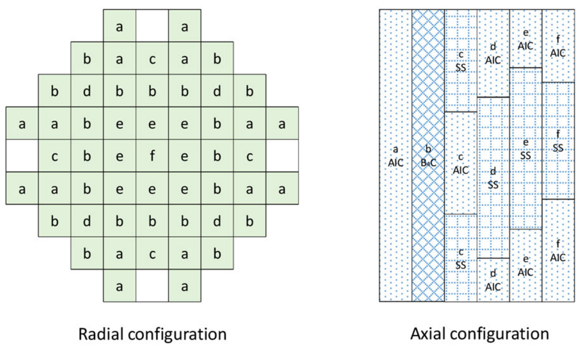

Figure 6. The radial and axial layout of the control rods of the KSMR core (AIC, SS, B_4C).

For the PARCS/SCF diffusion pin-by-pin simulation, the pin-homogenized cross-section is generated with Serpent2 and the Super Homogenization (SPH) method [31]. at Hot Zero Power (HZP) condition. The initial state and the key transient parameters are given in Table 2.

Table 2. The initial and transient parameters of the REA in KSMR.

Initial power (ratio to nominal) (-)	1.0E-6
Initial fuel temperature (K)	569
Initial coolant temperature (K)	569
Duration time (sec)	0.05
Total transient time (sec)	3.0

The power evolution during the REA is given in Figure 7. The power starts from 10-6 of nominal power, reaches the peak power of ~7 times nominal power at 0.14s, and falls back to 10-2 of nominal power at the end of the transient.

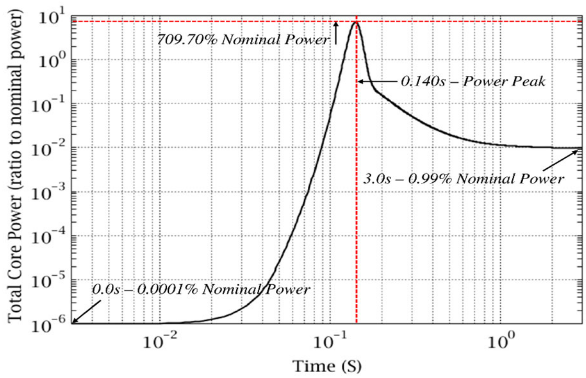

Figure 7. Power evolution during the REA transient in KSMR predicted by pin-level PARCS/SCF.

4.3. CAREM Core Analysis with Serpent2/SCF at pin/subchannel level

The CAREM-like core [38] was analyzed with Serpent2/SCF. The core is composed of 61 hexagonal fuel assemblies (FA) loaded with UO_2 enriched with either 1.8% or 3.1%. It consists of four different FAs, which differs from each other in enrichment and number of burnable poisons (BP). The control rod banks are distributed in the core in groups of three, except the one in the middle. The Serpent2/SCF model includes all the details of the FAs without approximations. Figure 8 shows the fuel-centered thermal-hydraulic SCXF-model, where 7747 rods and 7747 subchannels are considered for the core. There, details of the SCF model at pin/subchannel level as well as the full 3D core representation with the core axial discretization are shown.

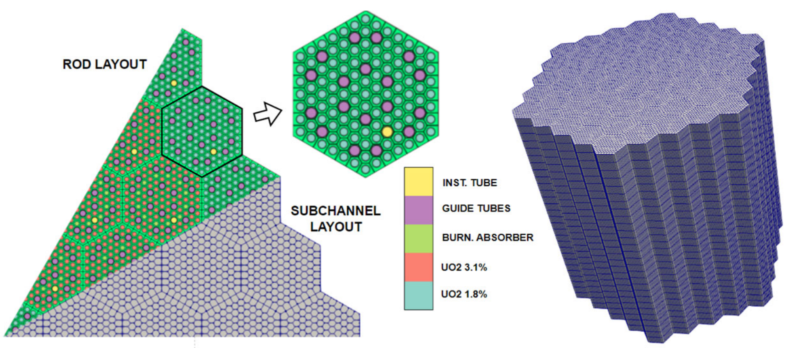

Figure 8. SCF model at pin/subchannel level. (Left) only 1/6 of the core is shown with the rod and subchannel layout details. (Right) Axial discretization of the core.

Figure 9 shows the pin power map distribution obtained from a steady-state simulation using Serpent2/SCF in a HFP state with a critical control rod bank configuration (control rod banks 1, 2, and

9 are partially inserted. The predicted core averaged radial pin map and the coolant temperature of each subchannels are presented Figure 10. More details and comparisons against nodal solutions can be found in [21].

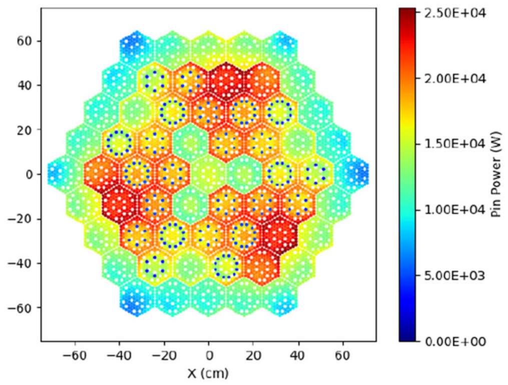

Figure 9. Axially integrated pin power map.

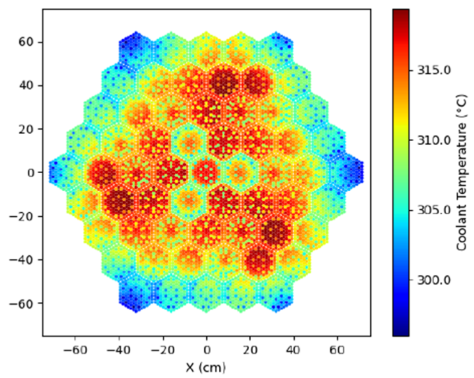

Figure 10. Axially averaged coolant temperature.

5. CONCLUSIONS

The code development and coupling activities at KIT for improved simulation of the neutronics and thermal hydraulic phenomena of water-cooled SMRs were presented and selected results were discussed. It includes both deterministic and stochastic codes for nodal/channel and pin/subchannel level simulations. These new computational tools will be step-by-step validated using experimental data when available since the validation is very important for their use in safety evaluations. It is worth to mentions, that the numerical tools are also applicable for large LWR and also to research reactors. The obtained results are very promising and encouraging for further improvements and applications.

6. OUTLOOK

Based on the achieved developments and implementations, the focus of the investigations in the next years will be on the following issues: a) Implementation of a time-dependent solution for the PARAFISH SP_N-solver for both static and transient analysis of SMR-transients at different spatial refinement (nodal/channel, pin/subchannel level), b) Implementation of an ICoCo-interface in PARAFISH for coupling with any thermal hydraulic solver equipped with a ICoCO-interface e.g., SCF And TPF, c) Explore different parallelization algorithms to be implemented in TPF and PARAFISH, and d) Extend the validation bases of the in-house codes.

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