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Verification of Neutronic and Thermal-hydraulic Multi-physics Steady-State Calculations for Small Modular Reactors with PARCS and TWOPORFLOW

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Abstract

In a nuclear reactor's core, different mechanisms and processes that determine the integrity of the safety barriers take place e.g. two-phase flow and heat transfer along the core height. In the case of Small Modular Reactors, the core is shorter and the fuel loadings are quite heterogeneous with a complex control rods designs. There is a need to evaluate the models of numerical tools and go beyond legacy codes by applying high fidelity, multi-physics and multi-scale approaches to predict safety parameters in normal operation and transient scenarios. PARCS is a computer code that solves the time-dependent two-group neutron diffusion equation in three-dimensional Cartesian geometry using nodal methods to obtain the transient neutron flux distribution. The code may be used in the analysis of reactivity-initiated accidents in light-water reactors where spatial effects may be important. It may be run in the stand-alone mode or coupled to other NRC thermal-hydraulic codes such as RELAP5. TWOPORFLOW is a KIT in-house developing code that solves in 3D Cartesian geometry the mass, momentum and energy conservation equations based on the two-fluid porous-media approach to describe the thermal-hydraulics of reactors cores. It can perform steady-state and transient calculations. In order to perform the coupling between PARCS and TWOPORFLOW the ICoCo interface was implemented in both codes for data exchange. A Small Modular Reactor core was modelled for testing the coupled code PARCS/TWOPORFLOW, this reactor core is based on the Korean Small Modular Reactor design called SMART, which is an integrated PWR. In this work, just the critical steady-state calculation is presented. Various neutronic and thermal-hydraulic parameters were compared against different coupled calculations. Good agreement between the results and references was achieved. In the future, transient calculations will be performed, having the goal of performing a Rod Ejection Accident at hot zero power conditions successfully.

1. INTRODUCTION

Over the last years Small Modular Reactors (SMRs) development has increased due to its emphasis on safety and passive systems, also its reduce power output is suitable for different electric grids. Various SMRs designs are being developed, but the trend is heading to Integrated Pressurized Light Water Reactors (iPWR), this means that the primary cooling circuit is within the Reactor Pressure Vessel (RPV). Some of these work with forced flow or with natural circulation, with or without boron, multiple alternatives are explored.

The System-integrated Modular Advanced Reactor (SMART) [1] is an advanced small-sized integral pressurized water reactor developed by Korea Atomic Energy Research Institute (KAERI). The SMART's reactor core, pressurizer, Steam Generators (SGs), and reactor coolant pumps are all integrated into a single RPV, as it is shown in Figure 1. This feature enabled large-sized pipe connection to be removed; thus, eliminating the possibility of a Large Break Loss of Coolant Accident (LB-LOCA). The SMART RPV houses four canned-motor pumps and eight helical-coiled SGs. The SGs in SMART are placed above the reactor core in order to provide enough coolant density gradients for establishing natural circulation inside the RPV in case of an accident. The working principle of the helical-coiled SGs is different from the U-tube design used in conventional PWRs. In the helical-coiled SGs, the primary coolant flows downward outside the helical-coiled tubes, whereas the secondary coolant flows upward inside the helical-coiled tubes, which is the opposite of U-tube SGs. Also, the coolant volume inside the helical-coiled tubes (i.e. coolant inventory of the SG's secondary-side) is much smaller than in U-tube SGs. Therefore, the thermal-hydraulic performance differs from using U-tube SG designs.

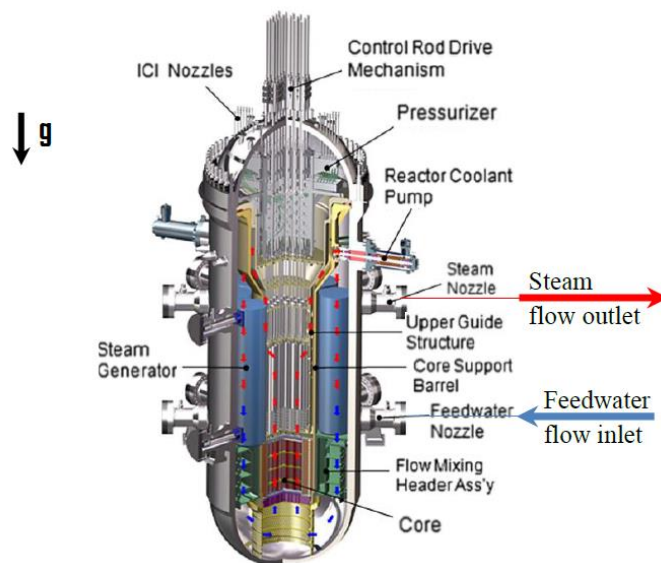


Figure 1. SMART's reactor pressure vessel and its internal components

The reactor core of SMART is designed to provide a thermal power of 330 MW_{th} with 57 Fuel Assemblies (FAs) that have an active length of 2 m (almost half of conventional PWRs) with slightly enriched uranium oxide (UO₂) of less than 5 wt%. Soluble boron and 25 rod cluster control assemblies are used to control core excess reactivity during operation and bring the core into a safe shutdown state. In order to reduce boron concentration during the SMART normal operation at the beginning-of-life, SMART FAs are loaded with a number of lumped burnable absorbers made of Gadolinia (Gd₂O₃) mixed with the UO₂ [1]. The general data of the SMART-plant is summarized in Table 1.

As the industry changes, the tools for reactor analysis have to change as well. Novel approaches for modelling the different phenomena occurring in a Nuclear Power Plant (NPP) have been

developed based on the multiscale and multiphysics methodologies for analysis. Decomposing the analysis domain in pieces that suit the calculation scope of a computational code is the main idea to perform code coupling calculations.

Table 1. General SMART data

<i>General plant data (Primary-side)</i>	
Rated reactor thermal power (MWth)	330
Gross plant electric output (MWe)	100
Number of steam generators	8
Steam generators type	Helical-coiled
Cooling mode	Forced circulation
Number of reactor coolant pumps	4
Rated primary flow rate (kg/s)	2090
Operating pressure (MPa)	15
<i>Core data</i>	
Core inlet mass flow rate (kg/s)	2006.4
Core inlet temperature (C)	295.7
Core outlet temperature (C)	323.0
<i>Fuel assembly data</i>	
Number of fuel assemblies	57
Lattice geometry	Square with 17x17 array
Active fuel height (m)	2.0
Fuel material	UO ₂
Cladding material	Zircaloy-4
Moderator/Coolant material	Light water
Burnable absorber material	Gd ₂ O ₃ -UO ₂
<i>Control rod data</i>	
Number of control rods	25
Absorber material	Ag-In-Cd

Sub-channel/Porous-media analysis can meet the requirements of high fidelity analysis within a reasonable computing time. For simulating fluid flow in presence of heat addition from a fuel rod, various approaches based on different number of fluid-phase models have been developed for LWRs. Single fluid (homogenous) or two fluids (liquid and gas) for two-phase flow approaches had been considered. For each consider fluid a set of conservation equations are solved. Each additional term, in terms of the number of phases to model, adds information on the cost of computational time. Although Computational Fluid Dynamics (CFD) approach provides a higher fidelity solution, it is still too expensive in terms of computational time.

Multi-physics simulations that take into account the coupling between neutronic and thermal-hydraulic phenomena are of great importance in reactor safety and design, in which the nuclear scientific community devoted special attention to improving their efficiency, accuracy, and

robustness. In this regard, different coupled neutronics and thermal-hydraulics codes for the reactor core analysis based on a sub-channel solver had been developed, such as DYN SUB [2], PARCS/CTF [3], and PARCS/SUBCHANFLOW [4]. Improve the prediction accuracy of the core behaviour taking into account the local feedbacks between undergoing core physical processes.

There exists different approaches for code coupling; the selected scheme for this work is external coupling with domain overlapping for multi-physics analyses. The Interface for Code Coupling (ICoCo) methodology has been chosen for data exchange between codes.

2. CODES

2.1 PARCS Code

PARCS is a three-dimensional (3D) reactor core simulator which solves the steady-state and time-dependent multi-group neutron diffusion or low-order neutron transport equations in Cartesian or hexagonal fuel geometries [5].

PARCS, as a stand-alone code, includes both a simple single-phase Thermal-Hydraulics (T/H) fluid model, which may be adequate for PWR analysis, and a two-phase T/H model called PARCS Advanced Thermal Hydraulic Solver (PATHS), which may be appropriate for Boiling Water Reactor (BWR) analysis. For models that require more sophisticated modelling of the T/H system behaviour, PARCS can be coupled with an external T/H system analysis code such as TRACE or RELAP5. PARCS has been directly integrated into the TRACE T/H code. However, for RELAP5, the Parallel Virtual Machine (PVM) package is required to handle the communication between the two codes.

The essential aim of PARCS modelling is to represent the physical reactor system with an approximate, but accurate, numerical model. The fundamental modelling aspects in the reactor kinetics calculation include the geometric representation, the cross section representation, and the T/H feedback modelling. PARCS provides a 3D geometric representation that can be reduced as necessary to 2D, 1D, or 0D by the choice of the appropriate boundary conditions. However, a special 1D kinetics capability is also available for more accurate and versatile 1D modelling.

PARCS has been extended to model not just typical Light Water Reactors (LWRs), but also Pressurized Heavy Water Reactors (PHWRs) and High Temperature Gas Reactors (HTGRs). Several additional modelling features have also been added to the code.

2.2 TWOPORFLOW Code

TWOPORFLOW (TPF) is a thermal hydraulic steady-state and transient porous-media two-phase flow code based on the coupled Euler equations for the liquid and vapour phase including friction with a solid medium. TPF solves six governing equations (3 for each phase); based on a finite volume method with a staggered grid configuration in three-dimensional Cartesian coordinates. The numerical solution method is developed from the Implicit Continuous Eulerian (ICE) method. For nuclear reactor applications is used for sub-channel calculations. It is written in FORTRAN 95 programming language [6].

As working fluid, only steam and water are included and the state equations based on IAWPS-formulation are implemented. A 2D heat conduction model is implemented for cylinder geometries where the Fourier's law equation is solved using a finite volume method considering the temperature dependent thermo-physical material properties. In TWOPORFLOW, a set of wall/fluid and inter-phase heat transfer correlations are implemented for a vertical flow regime covering the whole pre-CHF range to close the system of conservation equations [7].

The velocities are defined at cell boundaries all other main variables are defined at cell center. Figure 2, show how variables are defined within a single cell of the 3D mesh of TPF.

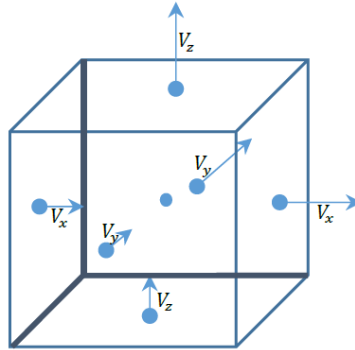


Figure 2: TPF single cell variables definition

2.2.1 Porous media approach

In the porous media approach, solid structures such as fuel rods are represented like blocking volumes and areas. The porosity is calculated based on the dimensions of the regular structures.

In order to calculate the thermal hydraulics in reactor cores, TWOPORFLOW needs the volume porosities (ϵ_V) as input. The calculation of ϵ_V in each cell is performed by dividing the volume of the fluid (V_F) by the total volume (V_T):

$$\epsilon_V = \frac{V_F}{V_T} \quad (1)$$

The hydraulic diameter in each cell is calculated by:

$$D_h = 4 \frac{A_{main}}{P_w} \quad (2)$$

where, P_w is the wetted perimeter and A_{main} the flow area in the main flow direction from bottom to top (z-coordinate) for structured porosity like reactor cores.

For rod arrangements the Cartesian discretization can be done in different ways e.g., centered rod, centered coolant (like in most sub-channel codes), or assembly wise where the whole assembly is seen as a channel, see Figure 3. In each case, each cell has to include one representative rod. So, the rod centered and assembly wise arrangement is the simpler one, because defining sub-channels between

the rods mean that the rod behaviour is averaged in maximum from four individual rods. In the case of a whole assembly, the included rods are averaged to one representative rod [6].

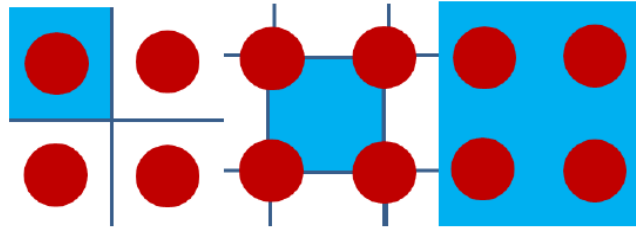


Figure 3: Different rod arrangements in channels

3. ICOCO COUPLING IMPLEMENTATION

3.1 ICoCo Description

The ICoCo interface defines how a “Problem” should behave. A Problem is seen like an object which computes a time dependent solution (result of equation solver), function of time dependent input data. The interface specifies methods that the problem has to provide and what they are supposed to do. It also specifies when and how these methods can be called. The supervisor performs the coupling algorithm: it calls methods on every problem and takes in charge interpolation and data manipulation, totally outside the coupled codes. Figure 4, shows the architecture of code coupling via ICoCo interface.

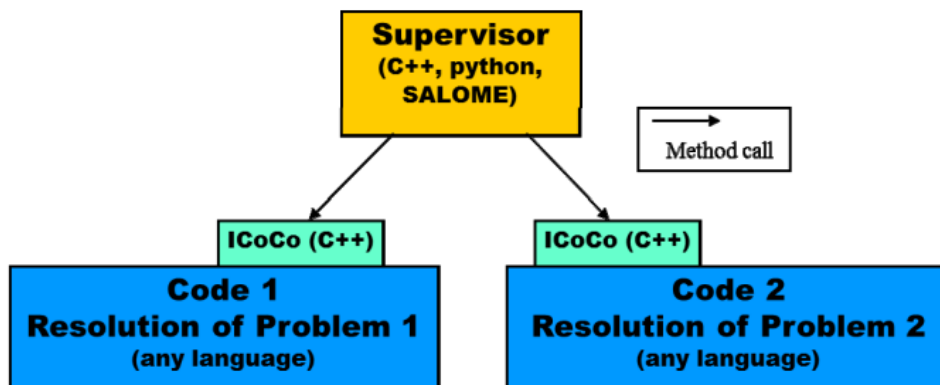


Figure 4: Overview of ICoCo architecture

ICoCo is written in C++ and defines mother classes which will control each code. ICoCo defines methods to a common mother class named “Problem” that allow initialization, time advance, saving and restoring, and field exchange [8].

3.2 Supervisor execution

The execution process of a code or a coupled code system through the ICoCo's Supervisor can be seen in Figure 5.

First of all, the supervisor has to instantiate the ICoCo problems which will control execution of the codes that have to be coupled. Then the supervisor can initialize the different problems with:

- *setDataFile*, if needed
- *setMPIComm*, if needed
- *initialize*.

The supervisor starts the time loop which will end after reaching the final time.

The computation time step is performed by *computeTimeStep* method, called for each interfaced code. The supervisor can use different time step for each code or use the same one (the minimum one for example). It depends on the coupling strategy. The selected computation time step is given to the code with *initTimeStep* method (same one for all codes or a different one by code).

The supervisor recovers the output fields to be exchanged from one code to another with *getOutputField* method. If needed, the fields can be changed before being injected into wanted code.

The input fields can now be passed to the codes through *setInputField* methods (after a call of *getInputFieldTemplate*).

The computations of each code are now performed on the current interval, using modified input fields through *solveTimeStep*. If everything is OK for each code, the computation can be validated through *validateTimeStep* method. If there is a problem with one of the codes, the computations are stopped through *abortTimeStep* method and another computation time step has to be performed and given to all codes.

Once the final time reached, the supervisor closes all the problems with:

- *terminate*
- *destructor*.

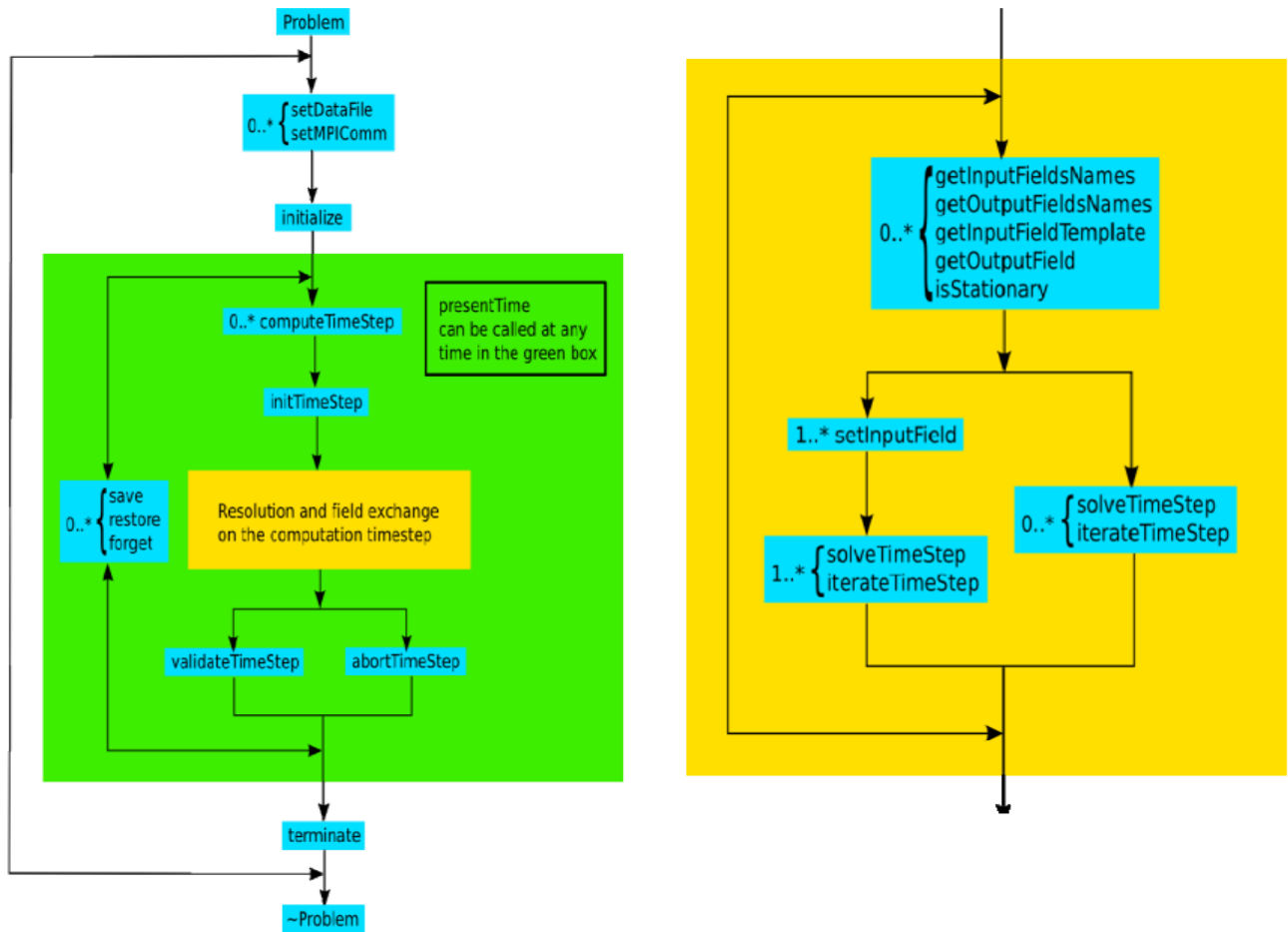


Figure 5: Execution flow chart using ICoCo interface

3.3 ICoCo Implementation in TWOPORFLOW

In this work only TWOPORFLOW's ICoCo implementation will be described, it has to be noted that the implementation process for other codes, e.g. PARCS, is very similar but, it may be some differences due to the intrinsic differences of the codes.

To implement the ICoCo interface to TWOPORFLOW, first, the original source code must be highly modularized; this was not a problem since the source code of TWOPORFLOW from scratch it is divided in FORTRAN 95 subroutines.

Then, the C++ Problem class *Problem2Porflow* was created according to the ICoCo standards. The ICoCo implemented methods for TPF are:

- Public methods:
 - *Problem2Porflow*()
 - *~Problem2Porflow*()

- Methods for initialization and termination:
 - *setDataFile()*
 - *initialize()*
 - *presentTime()*
 - *terminate()*
- Methods for time advance:
 - *solveSteadyState()*
 - *computeTimeStep()*
 - *initTimeStep()*
 - *solveTimeStep()*
 - *validateTimeStep()*
- Methods for getting field from the code and setting fields to the code:
 - *getInputFieldNames()*
 - *getOutputFieldNames()*
 - *setInputMEDField()*
 - *getInputMEDFieldTemplate()*
 - *getOutputMEDField()*

The mesh for TPF is an unstructured mesh created with TPF input parameters, during the Supervisor execution it is created when the *initialize* method is called. Two meshes are created for data exchange:

- 2D_SUB
- 3D-SUB

The MED fields are written in these meshes depending on the usage, for boundary conditions the field is written in the 2D_SUB mesh, and for source terms the field is written in the 3D_SUB mesh.

For interaction between the C++ ICoCo wrapper and the FORTRAN TPF solver some intermediate FORTRAN subroutines were created, these subroutines deals with the ICoCo methods calls. The created subroutines are:

- *icoco_cptimestep.f90*
- *icoco_creatMesh.f90*
- *icoco_fieldio.f90*
- *icoco_init.f90*
- *icoco_initTimeStep.f90*

- icoco_setdatafile.f90
- icoco_solve_steady_state.f90
- icoco_validate.f90

The exchange fields are set into TPF via one subroutine called *update_icoco.f90*, this subroutine is called within TPF calculation and only a few lines of code are added to the original source code to achieve data exchange between TPF and ICoCo. The FORTRAN module *icoco_globals.f90* for defining the ICoCo variables was added to the main source code. With these few changes of the original source code the maintenance of the ICoCo implementation can be easily done.

4. KARLSRUHE SMR (KSMR) CORE’S MODEL DESCRIPTION [9]

The basic fuel assembly design is based on the well-proven PWR technologies of 17x17 fuel rod arrays with 24 guide tubes and a central instrumentation tube. Since the developed core does not use soluble boron for reactivity control during normal operation, FAs are designed with fixed burnable poison rods. Each FA has either 20 or 24 burnable poison rods depending on their location in the core. These burnable poison rods are designed with an objective of reducing the hot full power excess reactivity at the beginning of cycle, and the power peaking in the core. To reduce the radial and axial power peaking factors, 6 FA-types are designed with radially and axially varying enrichment and burnable poison loadings. Figure 6 shows the KSMR fuel assemblies core distribution.

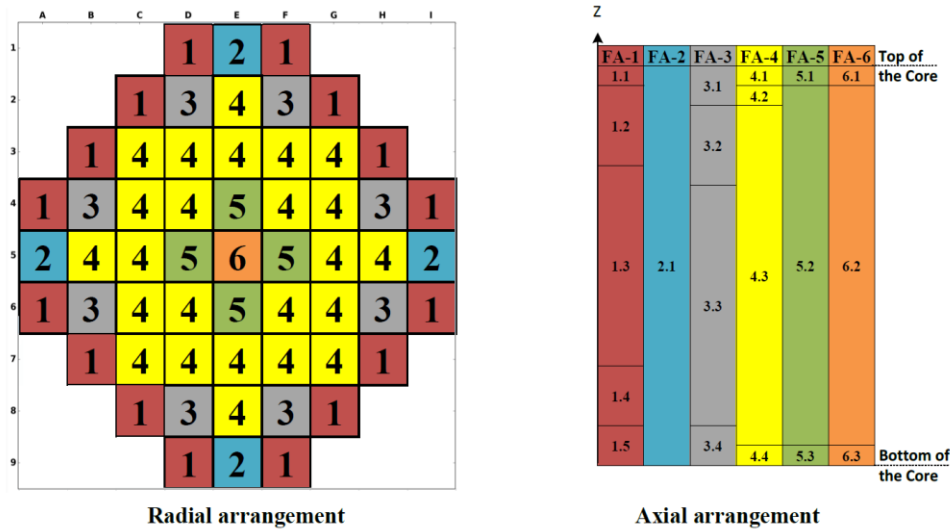


Figure 6: Fuel assembly types and distribution in the core

The control rods are designed and arranged to have three main functionalities: rapid negative reactivity insertion as a mean of providing enough shutdown margins, coarse, and fine reactivity adjustment for power manoeuvring and transient compensation. The developed core has 53 rodged fuel assemblies arranged into two banks: regulating and safety shutdown banks. The regulating

banks consist of 33 rodged fuel assemblies: 16 Ag-In-Cd control rods for coarse reactivity control and 17 hybrids control rods made from both Ag-In-Cd and stainless steel for fine reactivity control and axial power shaping. The safety shutdown banks consist of 20 control rods made of B₄C in fully extracted position during normal operation, and its goal is to provide enough and fast shutdown mechanism. The critical control rods configuration at hot full power condition is presented in Figure 7.

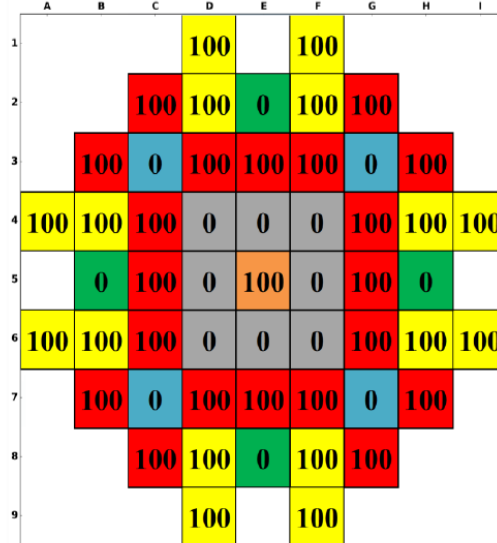


Figure 7: Critical HFP control rod configuration

5. STEADY-STATE CALCULATIONS

Steady-state calculations were performed with the parameters shown in Table 1 the model was presented in the previous section. For this calculation the investigated core parameters were: maximum coolant temperature, average coolant temperature, Doppler temperature, and coolant density.

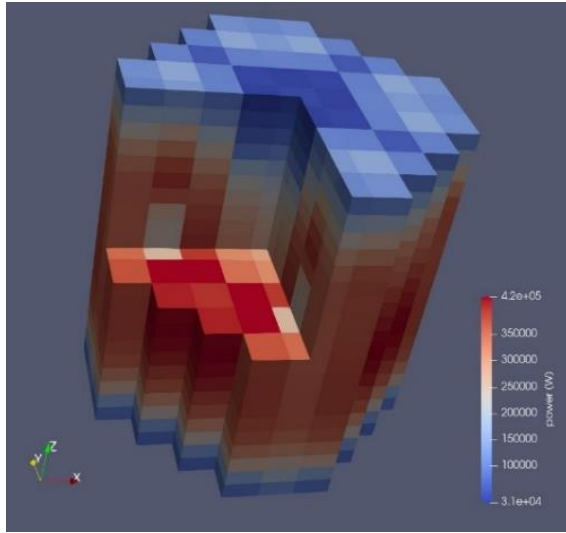
For results comparison, design parameters of KSMR core and the calculations of the coupled system PARCS/SUBCHANFLOW were selected, this coupled system is used as reference for code to code comparison since it is been applied within MCSAFER Project [10]. Table 2 gathered the results for the selected parameters. From design features, the coolant temperature raise within the core is 28 C, with PARCS/TPF this value is 27 C.

Table 2: Results comparison between PARCS/SCF and PARCS/TPF

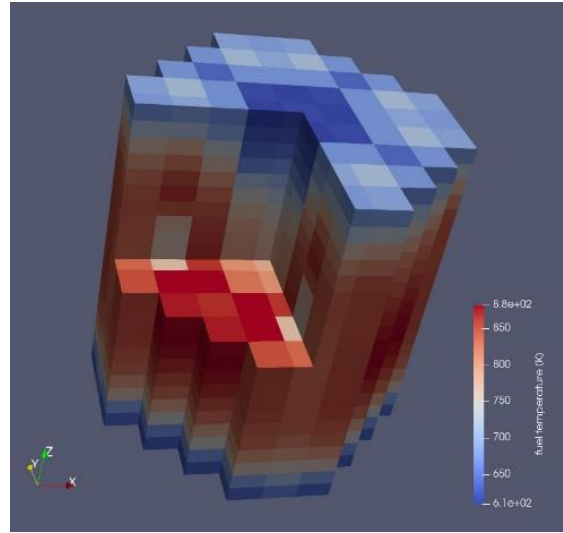
<i>Parameter</i>	<i>PARCS/SCF</i>	<i>PARCS/TPF</i>	<i>Difference*</i>
Max. coolant temp (K)	604.5	603.8	0.1157
Avg. coolant temp (K)	584.5	584.3	0.0342
Doppler temp (K)	817.0	789.7	3.3414
Coolant density (g/cm ³)	0.69892	0.69988	-0.1373

$$* \frac{SCF-TPF}{TPF} \times 100$$

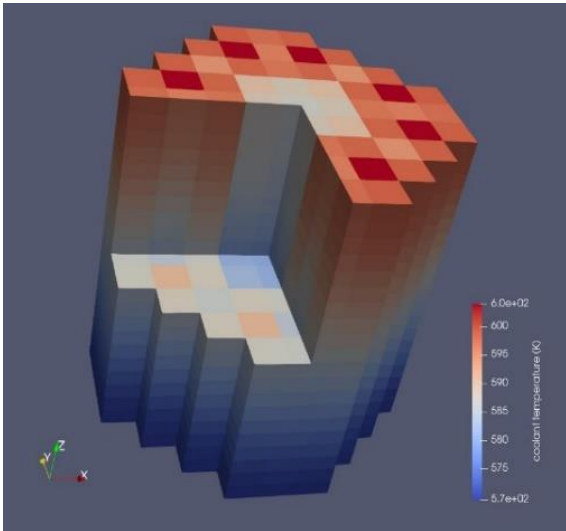
From Table 2 it can be appreciated a difference of 3.3% between de Doppler temperature values, it is due to the nature of the value itself. In SUBCHANFLOW (SCF) the Doppler temperature is a weighted average between the fuel surface temperature and the fuel center temperature. Meanwhile, in TWOPORFLOW the Doppler temperature is a volume average rod temperature. However if we look to the other values is clear that both calculations are close, with differences around 0.1%. Figure 8, shows the local distribution of power (Figure 8a), coolant temperature (Figure 8b), fuel temperature (Figure 8c), and coolant density (Figure 8d). It can be seen how all of these parameters are deeply related; power and fuel temperature distribution follow the same trend, in the same manner coolant temperature and coolant density are inverse proportional.



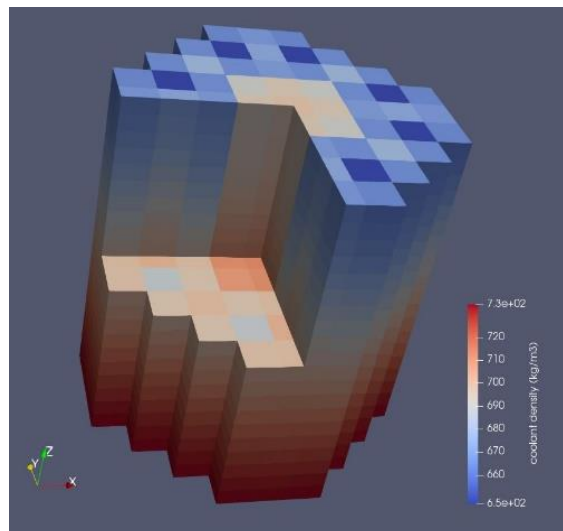
b) Power



a) Fuel temperature



d) Coolant temperature



c) Coolant density

Figure 8: 3D distribution of neutronic and thermal-hydraulic parameters

5. CONCLUSIONS

In this work was presented the Interface for Code Coupling (ICoCo) methodology to perform multi-physics neutronic and thermal-hydraulic calculations. In particular a detailed explanation of ICoCo's implementation in the thermal-hydraulic code TWOPORFLOW was described. Although no detailed explanation of ICoCo's implementation in the neutronic code PARCS was given, this work contributed to its verification. It can be concluded that ICoCo implementation in both codes was successfully done. Also, the coupled system exchange 3D data fields in a consistent way through the MED meshes created by ICoCo.

The KSMR model based on SMART small modular reactor was successfully developed in both codes, PARCS and TWOPORFLOW. The steady-state coupled calculation of PARCS and TWOPORFLOW shown good agreement with global design parameters. Steady-state results were compared against PARCS and SUBCHANFLOW coupled calculations, showing good agreement between both simulations.

Analysing 3D fields distribution it can be seen that power distribution, provided by PARCS, leads to a non-uniform radial coolant temperature profile. In this sense, it can be concluded that in the coupled case the power distribution calculated by PARCS and sent to TWOPORFLOW is better than the one that someone can model with the native TWOPORFLOW capabilities for input power distribution. The other way around, TWOPORFLOW coolant and fuel temperatures distributions provided to PARCS are better than what someone can model with native PARCS neutronics models. Which leads to a more accurate simulation.

With the achieved results, confidence is gained towards further development following ICoCo coupling methodology. Future work will be to performed transients where are strong neutronic and thermal-hydraulic feedbacks, e.g. rod ejection accident.

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