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Coupled serpent/subchanflow analysis with unstructured mesh interfaces for a hexagonal, plate-type VVR-KN fuel assembly

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This work presents the further development and application of the multi-physics coupled code Serpent/subchanflow for analyzing cores loaded with fuel assembly designs characterized by complex geometries, such as the VVR-KN fuel assembly. A high-detail steady-state analysis of one VVR-KN fuel assembly is presented and discussed. The VVR-KN is a plate-type fuel assembly, arranged coaxially with hexagonal fuel-plate tubes. Its particular geometry layout configuration challenges both their neutronic and thermal-hydraulic modeling. In this work, the versatility of Serpent's multi-physics interface is exploited by using the unstructured mesh-based interface to update the properties of the fuel and coolant materials in a coupled neutronic/thermal-hydraulic simulation; these properties are solved and provided by the thermal-hydraulic code Subchanflow. Both neutronic and thermal-hydraulic models are developed for a single fuel assembly of 6.83 cm distance pitch and 60 cm active height, and state conditions for the simulations are defined. Typical material composition and main thermal properties for the fuel-meat (UO₂-Al) and aluminum cladding (SAV-1) materials are extracted from references. This work paves the way for multi-physics analysis of research reactors with non-regular plates or subchannel geometries.

KEYWORDS

Monte Carlo, multi-physics, serpent, subchanflow, VVR-KN, unstructured mesh-based interface, research reactors

1 Introduction

In the last decade, considerable research and development was carried out worldwide to develop multi-physics coupling strategies to enhance the prediction accuracy of reactor physics simulations. This multi-physics strategy mainly involves the interaction between neutronics, thermal-hydraulics, and fuel performance codes, profiting from the great versatility of Monte Carlo neutronic codes and today's availability of powerful high-performance computing environments.

The Karlsruhe Institute of Technology (KIT) was leading different European projects, e.g., HPMC (High-Performance Monte Carlo Methods for Core Analysis) (Demazière et al., 2020), McSAFE (High-Performance Monte Carlo Methods for SAFETY Analysis) (Sanchez-

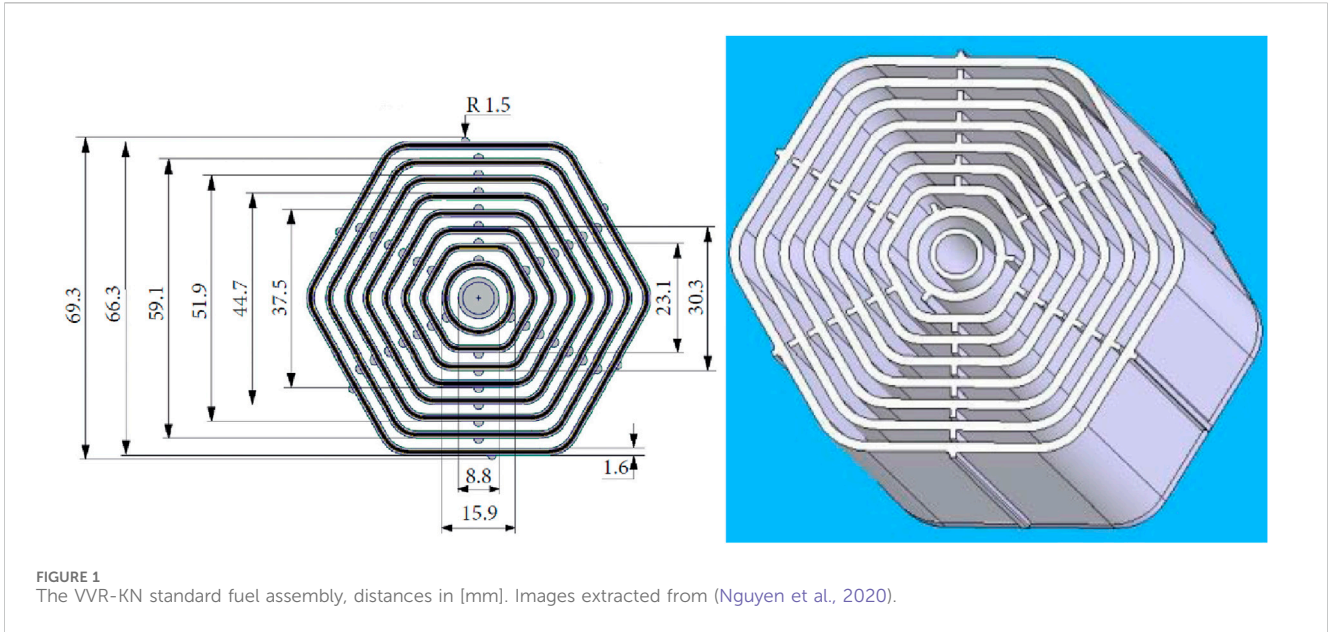


TABLE 1 Imposed TH conditions for stand-alone neutronic simulations.

Material	CZP		HFP(Xe = 0)	
	T [°C]	ρ [g/cm ³]	T [°C]	ρ [g/cm ³]
Meat	27	Table 3	70.0	Table 3
Cladding	27	Table 3	70.0	Table 3
Coolant	27	0.99657	53.4	0.98649

Espinoza VH. et al., 2021), and McSAFER (High-Performance Advanced Methods and Experimental Investigations for the Safety Evaluation of Generic Small Modular Reactors) (Sanchez-Espinoza VH. et al., 2021), where the proof-of-concept, development, optimization, and the verification and validation of multi-physics coupling strategies based on Monte Carlo neutronics for Light Water Reactor applications were performed and demonstrated. These efforts are paving the way for their use in more industry-like and safety relevant applications (Sanchez-Espinoza VH. et al., 2021). In this framework, the coupling between Serpent and Subchanflow based on an internal master-slave approach was developed (Ferraro et al., 2020a). The coupling has been widely tested under different benchmarks such as steady-state analysis on a full VVER-1000 core (Ferraro et al., 2021a), burnup analysis on PWR and VVER fuel assemblies (Ferraro et al., 2021b), and reactivity insertion transient problems on Pressurized Water Reactors (PWRs) (Ferraro et al., 2020b; Ferraro et al., 2020c) and Small Modular Reactors (SMRs) (Mercatali et al., 2023; Huaccho et al., 2025). Additionally, the KIT code Subchanflow developed initially for rod-type fuels has been modified and extended for the thermal-hydraulic analysis of thin plate-type fuels widely used in Material Testing research Reactors (MTRs) (Almachi et al., 2021). With this new extension in Subchanflow, the Serpent/Subchanflow tool has been used additionally to perform steady-state and transient simulations in some MTR-type cores such as the generic IAEA 10MW MTR core

TABLE 2 Boundary conditions for the TH feedback.

Parameter	Value
Power [kW]	393.49
Coolant inlet temperature [°C]	45.0
Core inlet pressure [kPa]	135.0
Coolant mass flow rate [kg/s]	5.58
Coolant's flow direction	Upward

(Almachi et al., 2022) and the SPERT IV D-12/25 core configuration (Almachi et al., 2024).

All the vast applications cited that use the coupling Serpent/Subchanflow rely in particular on one type of multi-physics interface, i.e., the regular mesh-based interface type 2 and the nested version type 22 (Serpent, 2024), which is perfect for modeling most of the standard reactor core designs. This work provides a first step in performing Serpent/Subchanflow coupled simulations using the unstructured mesh-based interface type 7 (Serpent, 2024). Interface type 7 was designed specifically to bring in solutions from solvers based on unstructured meshes such as fluid dynamic (CFD) codes. Its generality for defining different mesh shape geometries makes it suitable for the analysis of more unique core designs.

The structure of this work is as follows: Section 2 presents a general description of the VVR-KN fuel assembly. Section 3 describes the problem and defines the state conditions for the simulations. Section 4 briefly describes the tools and their main characteristics for simulating a coupled problem. Section 5 presents a detailed description of the neutronic and thermal-hydraulic models together with the interfaces based on unstructured meshes. Section 6 presents selected neutronic and thermal-hydraulic results. Finally, section 7 presents the summary and main conclusions of the work.

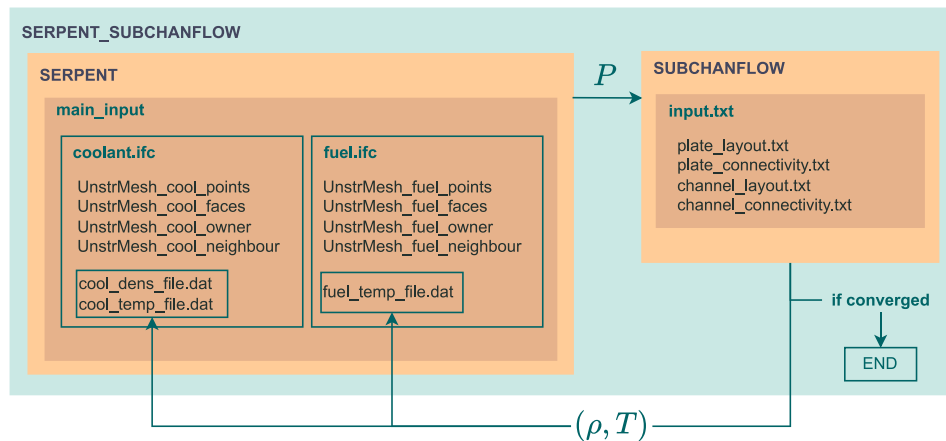


FIGURE 2 Flow calculation for a steady-state simulation with Serpent/Subchanflow using unstructured mesh-based interfaces for coolant and fuel. UnstrMesh_cool_* and UnstrMesh_fuel_* files define the unstructured superimposed meshes to update coolant and fuel properties.

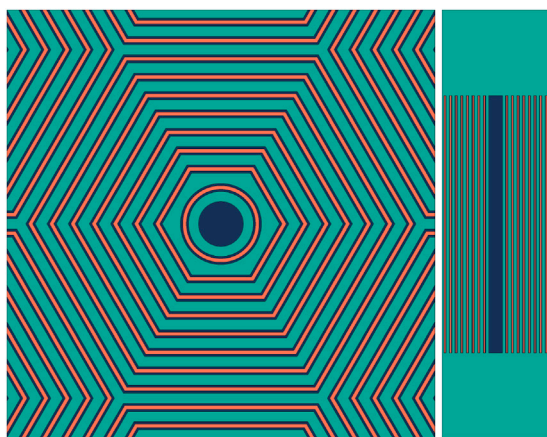


FIGURE 3 Radial and axial cuts from the Serpent model.

2 The VVR-KN fuel assembly

The VVR-KN is a hexagonal plate-type Russian fuel assembly design used in some research reactors. It comprises eight coaxial fuel elements (FE), seven having a hexagonal cylindrical shape, as showed in Figure 1. It has a characteristic pitch distance of 6.83 cm and 60 cm active height. The fuel meat is made of a UO₂-Al mixture, with a uranium density of 2.8gU/cm³ enriched in 19.75% of U₂₃₅ (Nguyen et al., 2020). The cladding and structural materials are made of SAV-1 aluminum alloy.

3 Problem definition

Imposed thermal-hydraulic (TH) conditions are defined for neutronics stand-alone characterization, and TH boundary conditions (BC) are defined for the steady-state neutronic/TH

TABLE 3 Fuel and cladding material composition.

Property	UO ₂ [63 wt.%]-Al		SAV-1	
Density [g/cm ³]	5.0432		2.88	
Composition [wt.%]	U ₂₃₅	10.965	Al	98.41
	U ₂₃₈	44.555	Mg	1.00
	O ₁₆	7.480	Si	0.44
	Al	37.000	Fe	0.14
			Cu	0.01

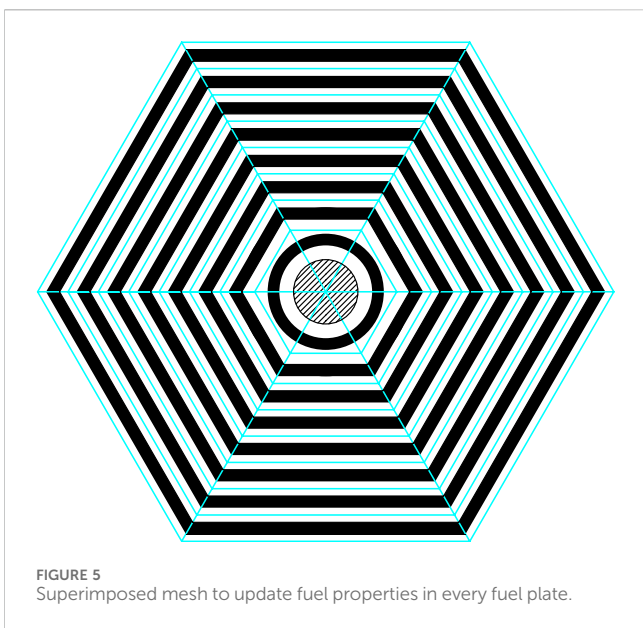
characterization. Most of the information needed for this work was extracted from (Nguyen et al., 2020). Two imposed TH states are defined, i.e., Cold Zero Power (CZP) condition and Hot Full Power (HFP) without xenon condition, see Table 1.

For the neutronic/TH characterization, boundary conditions for the TH feedback are defined considering nominal operation conditions. The reference values were obtained from (Nguyen et al., 2020), where a 10 MW conceptual core design using VVR-KN fuel assemblies (FAs) was investigated, and a maximum power of 393.49 kW is reported for a single FA. This power is considered as a reference value, and additional BCs are summarized in Table 2.

4 Multiphysics tools

4.1 Serpent

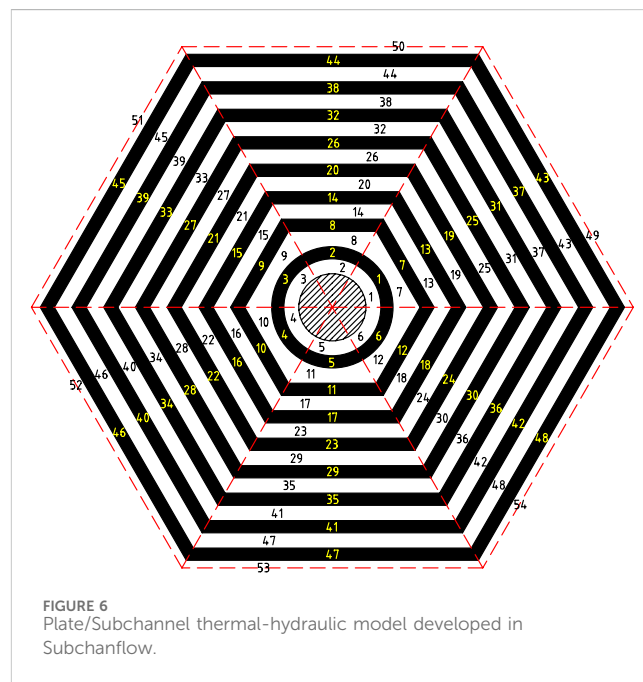
Serpent is a multi-purpose, three-dimensional, continuous-energy Monte Carlo transport code developed since 2004 at VTT Technical Research Centre of Finland Ltd (Leppänen et al., 2015). It represents a state-of-the-art code aimed to perform static, burnup, and dynamic 3-D calculations using standard ACE format Nuclear Data Libraries. Serpent was originally developed as a reactor physics



code, but the scope has considerably broadened over the years, bringing the development of many advanced features (Serpent, 2024). One of those main advanced features is the multi-physics (MP) capability (Valtavirta, 2015). The basic idea of the Serpent's MP capability is to bring certain material properties into the Serpent model, e.g., material's density and temperature distribution, in order to have more realistic modelling during the simulation. The MP feature is wisely designed by an interface, which is defined on top of the Serpent's model, i.e., without altering the original model's geometry. Depending on how the external code solves the problem in terms of physics and geometry discretization, different interfaces are available in Serpent, i.e., point-wise, rectangular and hexagonal regular meshes, unstructured meshes,

TABLE 4 Summary of the generated unstructured meshes.

Mesh parameter	Coolant mesh	Fuel mesh
Total cells or elements	1,080	960
Number of points	1,155	1,029
Number of faces	3,294	2,928
Number of neighbours	3,066	2,712



and many more. Examples of external codes coupled with Serpent via the MP interface are fluid dynamic (CFD) codes, channel thermal-hydraulics, and fuel performance codes (Leppänen et al., 2023; Leppänen, 2013).

One of the interfaces of interest for this work is the one based on unstructured meshes, designed specifically to bring in solutions from solvers based on this type of mesh. The interface is based on point-face-cell hierarchy, where the user gives a number of points that can be combined into a set of planar faces, which make up a set of closed convex cells (Serpent, 2024). The interface definition is based on the OpenFOAM format, and there is support for tetrahedral, hexahedral, and polyhedral-type meshes (Valtavirta, 2015). The Serpent version 2.1.32 is used in this work.

4.2 Subchanflow

Subchanflow (SCF) is a subchannel three-equations and single-phase flow thermal-hydraulic code for steady-state and transient analysis developed at Karlsruhe Institute of Technology (KIT), Germany (Imke and Sanchez, 2012). Subchanflow solves mass, momentum, and energy conservation equations along the axial discretization and between the neighbour lateral channels,

TABLE 5 Fuel and cladding thermal properties.

Property	Fuel	Cladding
Material	UO ₂ [63 wt.%]-Al	SAV-1
Conductivity [W/m/K]	64 (Abdukadyrova et al., 2014; Hagrman and Reymann, 1979)	151 (Abdukadyrova et al., 2014)
Specific heat [J/kg/K]	456 (Stahl, 1982)	924

TABLE 6 Global criticality results. The number in parenthesis is the 1σ uncertainty in the *k_{eff}*'s last digit. (*) imposed TH conditions.

Codes	Serpent		Serpent/SCF
	CZP	HFP	HFP
<i>k_{eff}</i> (1σ)	1.52968(8)	1.52585(8)	1.52577(8)
Ave. T _{fuel} [°C]	27*	70.0*	74.9
Ave. T _{clad} [°C]	27*	70.0*	73.4
Ave. T _{cool} [°C]	27*	53.4*	53.6

i.e., cross-flow between channels. These equations together with a set of empirical correlations to calculate, for example, the pressure drop, heat transfer coefficients, void generation, etc., represent the system of equations of the single-phase (liquid/vapor mixture) flow model (Imke and Sanchez, 2012). Subchanflow was initially developed for rod-type fuel elements, where the geometry is defined as a set of channels and rods with given hydraulic parameters and connectivities. A typical channel is characterized by its area, wetted and heated perimeter, and a list of its neighbour channels; and a typical rod is characterized by its material type for fuel and cladding, rod diameters and gaps, and a list of neighboured channels where the heat is released. The temperature profile inside each rod is calculated by dividing it into several radial rings and solving the heat equation in the radial direction by a finite volume method (Imke and Sanchez, 2012). An extension to plate-type fuel assemblies typically for analyzing MTR research reactors is also available in Subchanflow (Almachi et al., 2021). The Subchanflow version 3.7.1 is used in this work.

4.3 The Serpent/Subchanflow coupling

The Serpent/Subchanflow coupling was developed in the framework of the McSAFE project (Sanchez-Espinoza VH. et al., 2021), and the main implementation aspects were first introduced in (Ferraro et al., 2020a). The coupling relies on the capabilities and advanced features of both codes, e.g., the multi-physics interface in Serpent to interact with other codes and the Subchanflow aptness to be used as an external library. The implementation consists of a high-level set of routines (coupling routines) developed in C language. The coupling routines manage open-door functions defined in the Serpent code, which allows the management of all main aspects of a coupled scheme. Subchanflow is included and used

TABLE 7 Converged power distribution in every FE. The numbers in parenthesis are the 1σ uncertainty in the value's last digit.

FE	Plates	Power	Volume	Power density
		[kW]	[cm ³]	[W/cm ³]
1	1–6	17.29(1)	18.868	916.2(4)
2	7–12	27.81(1)	31.281	889.2(3)
3	13–18	36.39(1)	41.756	871.5(3)
4	19–24	45.01(1)	52.232	861.7(2)
5	25–30	53.65(2)	62.707	855.6(2)
6	31–36	62.38(2)	73.183	852.5(2)
7	37–42	71.07(2)	83.658	849.5(2)
8	43–48	79.88(2)	94.133	848.6(2)

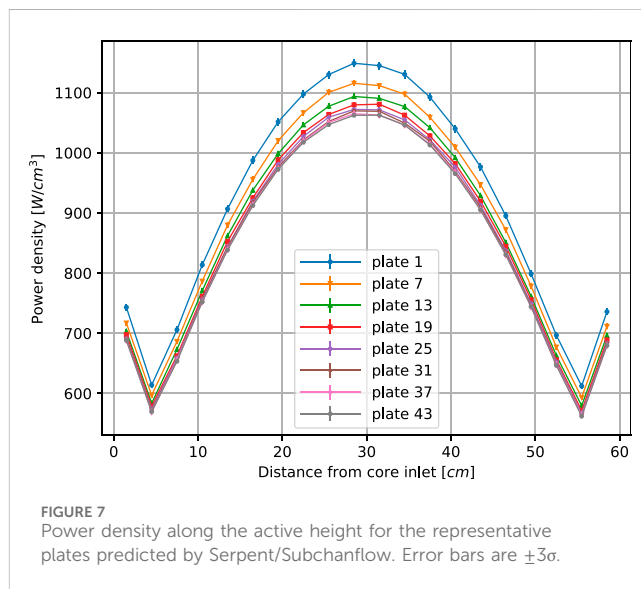


FIGURE 7 Power density along the active height for the representative plates predicted by Serpent/Subchanflow. Error bars are ±3σ.

as an external library, resulting in an embedded master-slave implementation (Ferraro et al., 2020a).

Figure 2 shows the flow calculation for a coupled steady-state simulation where successive iterations between Subchanflow and Serpent are performed. The codes exchange the Density-Temperature distribution (ρ, T)¹ and Power distribution (P) until a desired convergence is achieved. In the original implementation with regular mesh-based interfaces (Ferraro et al., 2020a), these variables are exchanged directly from RAM memory, i.e., copying the (ρ, T) variables to Serpent using the C function `memcpy()`; meanwhile, in this case, densities and temperatures (ρ, T) are overwritten in their respective interfaces files in every iteration, as shown in Figure 2. Only extra lines using

1 For simplicity, (ρ, T) denotes the fuel and coolant Temperature-Density distribution.

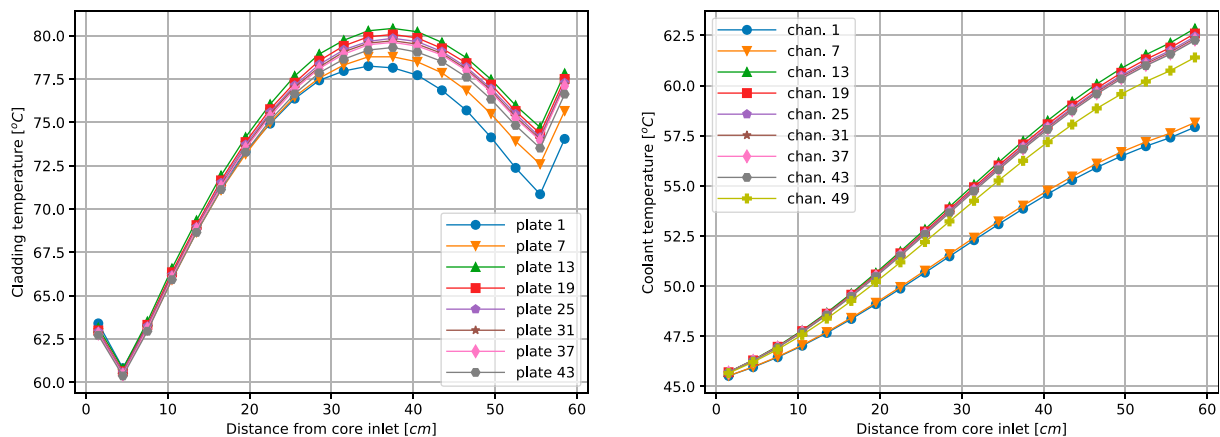


FIGURE 8 Cladding and coolant temperatures along the active height for representative plates and channels predicted by Serpent/Subchanflow.

fprintf() functions were needed in the coupling routines (Ferraro et al., 2020a) to accomplish this idea without affecting the Serpent and Subchanflow source codes.

5 Developed models

5.1 Serpent model

Following the fuel assembly description in Section 2, a 3D model was developed in Serpent as shown in Figure 3. The main assumptions and considerations taken into account are the following:

- A simplified model in terms of geometry was considered, i.e., no structural ribs, straight plate corners instead of curved ones, and a solid rod of SAV-1 material for the inner structural tube; see Figure 3.
- Pure water was considered for the bottom and top axial reflectors. Each with a 20 cm axial length. For the HFP state, fixed densities and temperatures corresponding to the inlet and outlet core temperatures are considered, i.e., 45°C and 62°C for the bottom and top axial reflectors, respectively.
- Most references related to this type of FA do not report the proportion between Aluminum and UO₂ in the meat. Only one reference that reports a volumetric concentration was found (Kkonoplev and Sorlov, 2010). In this work, a weight concentration of 63wt.% UO₂ in the meat was considered. A typical composition for an SAV-1 alloy was extracted from (Abdukadyrova et al., 2014; Salikhbaev et al., 2009). Table 3 summarizes the composition of both materials used in this work.
- JEFF-3.1.1 ACE nuclear data library was considered for the simulations. For the thermal scattering law of H in H₂O, generated libraries at 294K and 324K were considered for the CZP and HFP, respectively, in neutronic stand-alone characterizations. For the steady-state case, interpolation

between the libraries at 294K and 374K was considered according to the temperature predicted by Subchanflow.

- Reflective boundary conditions in the radial (XY) direction and black in the axial (Z) direction.
- For Serpent criticality simulations, 10³ cycles with 10⁵ particles each were considered, with 100 inactive cycles for source convergence.
- No xenon concentration was considered in the HFP state condition.
- Two independent meshes were generated using the MP interface type 7 to update the properties of the fuel and coolant materials. The meshes were created with the condition that a mesh cell encloses part of the material (meat or coolant) that is intended to be updated. For that, the FA was subdivided into six triangles, every triangle containing eight fuel plates and nine coolant subchannels. Figures 4, 5 show a 2D representation of each mesh. Axially, the active height was divided into 20 axial cells. Only the active height was considered for the TH feedback. Table 4 summarizes the characteristics of each mesh.

5.2 Subchanflow model

A thermal-hydraulic model at plate/subchannel level is developed in Subchanflow taking into account the following assumptions and considerations:

- The subchanflow model consists of 54 subchannels and 48 plates, and both subchannels and plates are divided axially in 20 cells, see Figure 6. Two subchannels surround every plate; for simplicity, the power generated in a plate is equally distributed to its neighboring subchannels.
- Dittus-Boelter and Colburn heat transfer correlations were considered. Blasius correlation for the friction factor, and the IAPWS-97 standard is selected for the coolant water properties.

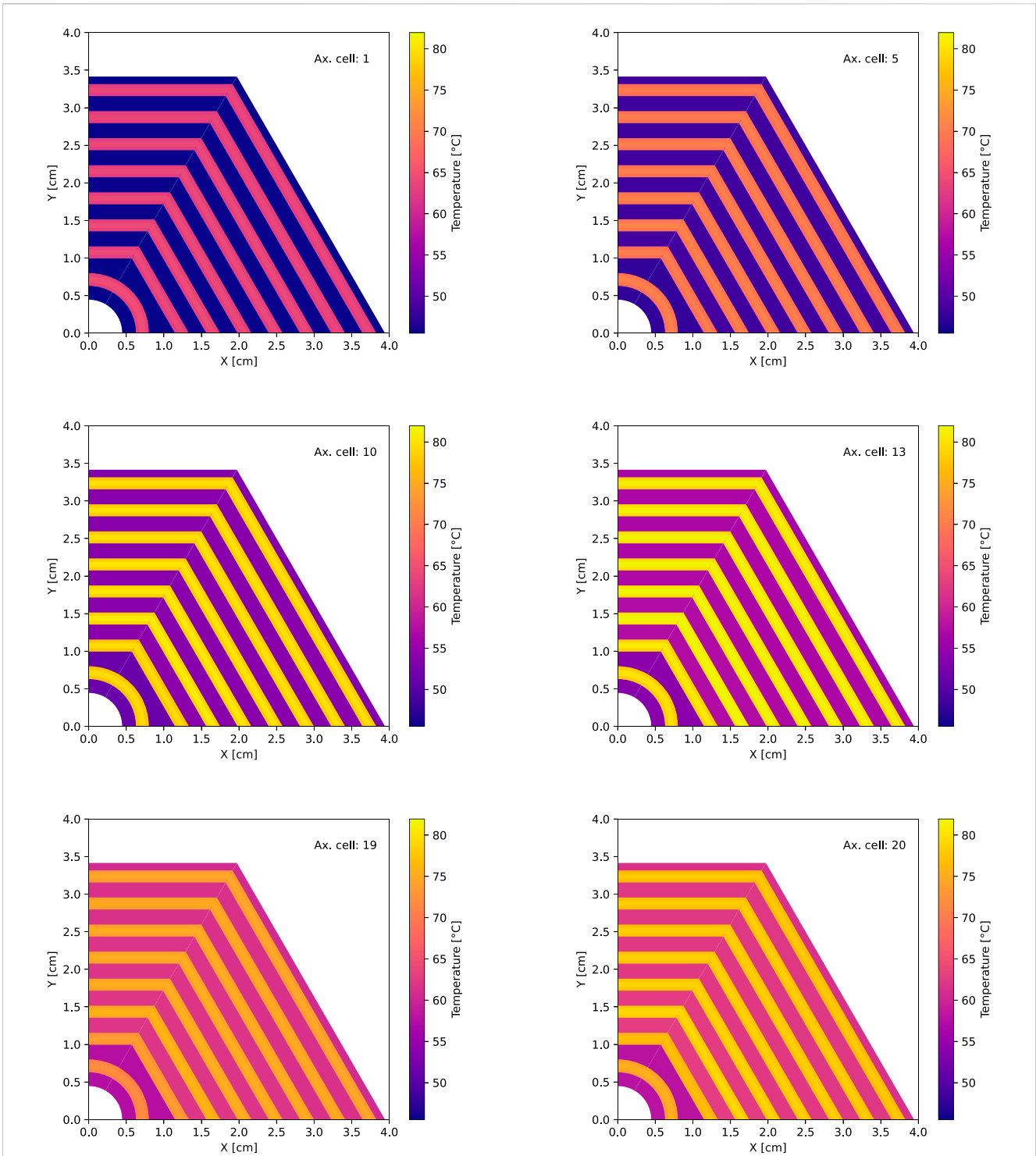


FIGURE 9 Temperature distribution predicted by Serpent/Subchanflow at different axial layers starting from the inlet to the core outlet. Only 1/4 of the core is shown due to the symmetry of the problem.

- For heat conduction in the fuel plate, five nodes were considered in the meat and two nodes in the cladding. Equivalent straight plates were considered for the inner circular fuel plate.
- Constant thermal properties showed in Table 5 were considered. The parameters were obtained considering a

- reference temperature of 70°C. Properties for UO₂ and Al materials were obtained independently, and weighted averages were considered using the mass fractions as weights. No thermal expansion in the materials was considered.
- Subchanflow calculates a temperature profile inside the thin fuel meat, and one single temperature value per cell is needed

TABLE 8 Serpent/Subchanflow steady-state simulations using different heat transfer correlations.

Parameter	Dittus-Boelter	Colburn	Diff.
$k_{eff} (1\sigma)$	1.52585(8)	1.52577(8)	3(4) pcm
Max. T _{fuel}	80.3°C	82.0°C	1.6°C
Ave. T _{fuel}	73.4°C	74.9°C	1.5°C
Max. T _{clad}	78.8°C	80.2°C	1.4°C
Ave. T _{clad}	72.1°C	73.4°C	1.3°C
Max. T _{cool}	62.9°C	62.9°C	0.0°C
Ave. T _{cool}	53.6°C	53.6°C	0.0°C

in Serpent for the fuel temperature feedback. A volumetric average value is considered for the cross-section adjustments in Serpent (on-the-fly temperature treatment (Viitanen and Leppänen, 2014)).

6 Results

Stand-alone neutronics and neutronic/TH simulations are presented in this section. All the simulations have been performed in a GNU/Linux single machine with an AMD EPYC 7542 32-Core Processor using 30 OpenMP threads. For the steady-state coupled simulation, eight iterations were performed, obtaining differences between the last two iterations in L_2 -norm (Ferraro et al., 2020a) of $< 9 \times 10^{-3}$ °C in fuel temperature, $< 7 \times 10^{-4}$ °C in coolant temperature, and $< 3 \times 10^{-7}$ g/cm³ in the coolant density. Every iteration took around 30 min, resulting in approximately 4 h to complete the steady-state simulation. A summary of the criticality results and average temperatures for the fuel (T_{fuel}), cladding (T_{clad}), and coolant (T_{cool}) are summarized in Table 6.

In the neutronics stand-alone results, a difference of ~ 160 pcm is observed as a difference between the CZP and HFP state conditions. No appreciable difference in reactivity is observed in the HFP state when the TH feedback is considered. The average temperatures predicted by Subchanflow are very close to the imposed temperatures for the HFP state, with a maximum difference of 4.9°C in the Ave. T_{fuel}.

Detectors to account for the power in every FE (Fuel Element²) are set up and summarized in Table 7. The higher power density is obtained in the internal FE and decreases slightly, keeping more or less constant in the remaining FEs. The axial power density distribution is shown in Figure 7. Thermal peaks due to the axial reflectors can be observed in both endings. A slight offset (almost negligible) of the axial power distribution in direction to the core inlet can be observed due to the slightly higher density of the coolant at the core inlet.

Figure 8 shows the axial cladding and coolant temperature distribution in representative plates and subchannels. The highest

cladding temperature is obtained in plate 13 (3rd FE), achieving a maximum value of 80.2°C in the 13th axial cell. The coolant temperature in channel 13 achieves a maximum value of 62.9°C in the last axial cell (core outlet). Figure 9 shows radial temperature distribution in all the materials (fuel, cladding, and coolant) at different axial layers.

The thermal-hydraulic results previously presented were calculated using the Colburn correlation. A sensitivity analysis comparing the Colburn and Dittus-Boelter correlations showed that the Colburn correlation yielded slightly higher temperature. To ensure a conservative approach, the results using Colburn were selected for presentation. The comparative results using these two correlations are summarized in Table 8, showing negligible differences, with temperature variations less than 2°C. The observed difference arises because the Colburn correlation predicts a lower heat transfer coefficient. This results in a higher temperature difference between the coolant and the external cladding surface, leading to slightly elevated cladding and fuel temperatures. Similar findings were reported during the Subchanflow validation for plate-type fuels (Almachi et al., 2021).

As a final step, a comparison against the TH evaluation performed in (Nguyen et al., 2020) is presented. The hottest FA producing 393.49kW is analyzed in both cases. However, different procedures are followed: The process followed in (Nguyen et al., 2020) consists first of a 10MW full-core characterization using the MCNP6 code, followed by a safety evaluation for the hottest FA in the core using the TH code PLTEM4.2 with detailed power distributions obtained from the core simulation. In our work, only the total power (393.49kW) was considered as an input for the single FA model in Serpent with reflective BCs, missing the real conditions of the FA in the core. Table 9 summarizes and compares some selected results. The Serpent/Subchanflow power distribution is more homogeneously distributed mainly due to the reflective BCs used in the radial direction, predicting a lower peak power value and, therefore, lower peak temperatures compared to (Nguyen et al., 2020) where higher peak power is predicted.

7 Summary and conclusion

A coupled neutronic/thermal-hydraulic simulation of a single VVR-KN fuel assembly using Serpent/Subchanflow was performed. Eight iterations were considered to obtain a converged steady-state solution, capturing consistent results regarding power and temperature profile distributions. Unfortunately, a comparison against experiments or referent simulations was hard to perform because of the simplified problem definition considered in this work and all the required assumptions, e.g., boundary conditions, set of correlations, material composition, and constant thermal properties. Nevertheless, the novelty of the result remains in the high-detail coupled neutronic/thermal-hydraulic solution in a non-regular plate or subchannel shape size, and it paves the way for a more realistic simulation, such as a VVR-KN full-core characterization.

An important remark of the work is the satisfactory use of the Serpent's unstructured mesh-based interface for the thermal-hydraulic coupling with Subchanflow. It is the first time that this type of interface has been employed within a Serpent/Subchanflow simulation. This interface type offers excellent versatility and more

2 The FA is composed of eight coaxially arranged FEs, and every FE in the thermal-hydraulic model is divided in six plates.

TABLE 9 Serpent/Subchanflow comparison against Nguyen work.

Parameter	Serpent/SCF	PLTEMP4.2 (Nguyen et al., 2020)
Max. Pdens [kW/cm ³]	1,150	1,442.6
Peak Power Factor	1.32	2.2
Max. Tfuel [°C]	82.0	-
Max. Tclad [°C]	80.2	83.0
Max. Tcool [°C]	62.9	66.0

generality for generating non-regular meshes. Minor changes in the coupling routines were required to ensure consistent data exchange between the two codes without affecting their source codes. A better performance could be achieved by exchanging the information directly from RAM memory. However, some changes in the source codes are needed to add this feature to the coupled tool.

Subchanflow has been validated widely for standard PWR and BWR rod-type fuels. However, extra development is still needed to enlarge the thermal-hydraulic analysis in MTR research reactors. Some examples of future developments are implementing critical heat flux correlations for plate-type fuels, temperature-dependent thermal properties for standard MTR materials, and heat expansion treatment.

Data availability statement

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

Author contributions

GH: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Software, Visualization, Writing—original draft, Writing—review and editing. TG: Conceptualization, Investigation, Software, Writing—review and editing. VS: Funding acquisition, Project administration, Resources, Writing—review and editing, Supervision. JA: Software, Writing—review and editing. UI: Software, Supervision, Writing—review and editing.

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