VERIFICATION OF A REACTOR PHYSICS CALCULATION SCHEME FOR THE CROCUS REACTOR

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Abstract

CROCUS is a zero power (100 W) reactor of the Laboratory for Reactor Physics and Systems Behavior (LRS) at the Swiss Federal Institute of Technology, Lausanne (EPFL). It is used for teaching and research purposes. In the CROCUS Safety Analysis Report (SAR), its modeling has relied on diffusion theory and point kinetics for the neutronic analysis and simplified thermal hydraulics models for accident analysis. Recently, an effort has started within the LRS to improve its modeling capabilities, the long term goal being to update the CROCUS SAR for improved operational flexibility.
The present work is focused on the static neutron analysis of CROCUS through the development of a 3D nodal simulator (e.g. PARCS) model of the reactor and its verification against reference solutions provided by either experiments or whole-core Monte Carlo calculations using the MCNP5 and SERPENT codes. The quantities of interest for the verification of the model are the k_{eff}, and the control rod worths.
Nodal core simulators are typically used in the industry for modeling of Light Water Reactors (LWR). The set of homogenized macroscopic cross-sections needed by the core simulator, referred in this work as nuclear data library, is generated by the SERPENT Monte Carlo code. An innovative homogenization approach to generate the nuclear data library is considered due to the irregular radial geometry of the CROCUS reactor.
PARCS k_{eff} predictions are within 400 pcm of the SERPENT/MCNP5 results, which in turn deviates by about 200 pcm from the experimental values. The latter deviation is covered by the uncertainty due to the nuclear data in the k_{eff} prediction (about 500 pcm). PARCS control rod worth prediction underestimates the reference solutions by about 30 pcm pointing towards necessary improvement in the homogenization procedure for control rods.

1. Introduction

CROCUS is a zero-power (100 W) teaching and research reactor of the Laboratory for Reactor Physics and Systems Behavior (LRS) at the Swiss Federal Institute of Technology, Lausanne (EPFL). The goal of the present work is to improveits in-house modeling capabilities; the long term goal being to update the CROCUS Safety Analysis Report (SAR) for improved operational flexibility. Because the long term goals involve the modeling of transients, a deterministic methodology based on the multi-step approach is chosen over the use of Monte Carlo methods.

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The multi-step approach consists of a set of transport calculations by a so-called lattice code on a subset of the geometry (typically a fuel assembly), in 2D and for various conditions (typically exposure, fuel temperature, void); followed by a 3D calculation done by a core simulator for a coarser discretization of the phase space (few energy groups, coarser spatial mesh, diffusion approximation, etc…). Monte Carlo methods are nonetheless used to provide a reference solution for steady-state analysis.

The paper is organized as follows. In the first section, a rudimentary introduction to the design of CROCUS is provided. In the second section, the various neutronic codes are presented and the CROCUS models are described. The third section is dedicated to the comparison of those tools. Finally, the last section of the paper summarizes the work performed and introduces the envisioned future work.

2. The CROCUS zero power reactor

The CROCUS zero-power teaching and research reactor (Figure 1) is a light water moderated facility licensed to a thermal power of 100 W (total flux of ~2.5 X 10^9 $n.cm^{-2}.s^{-1}$). The active core is approximately 60 cm in diameter and 100 cm in height and comprise of two different fuel zones. The facility operates at room temperature using a controlled water loop passing through two heat exchangers or an electrical heater when needed.

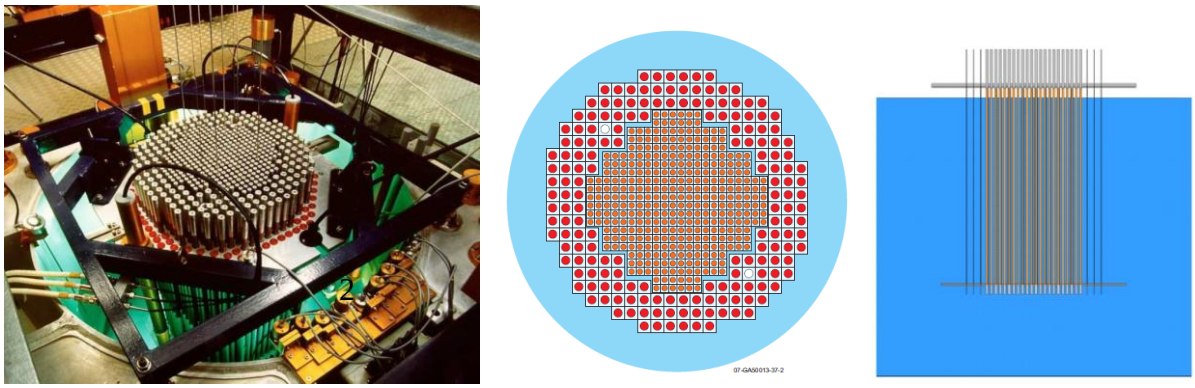


Figure 1 Top and side view of the CROCUS reactor showing the water tank and the two fuel lattices

The fuel rods are held in a rectangular lattice geometry between two octagonal stainless steel grid plates, each of which has a thin Cd layer to limit axial neutron leakage. The inner UO_2 zone consists of 336 fuel rods (pure Al cladding) with an enrichment of 1.806 wt.% of U-235 and a pitch of 1.837 mm. The outer zone consists of 176 metallic uranium fuel rods with an enrichment of 0.947 wt.% and a pitch of 2.917 cm. The total length of each fuel rod is 120 cm with an active fuel height of 100 cm. The core is placed in an Al-6060 grade vessel of ~132 cm in diameter and ~164 cm in height.

The reactor possesses two independent shut down mechanisms allowing it to be brought to a sub-critical state in less than one second. There are two cruciform shaped Cd blades at the core center and four safety tanks operated by a valve system to drain the moderator quickly. The

actuation of anyone of the six mechanisms is enough to shut down the reactor. The core reactivity is controlled by variation of the water level with an accuracy of ± 0.1 mm (equivalent to ± 0.4 pcm) and/or by means of two control rods (accuracy of ± 0.3 mm or ± 0.2 pcm) containing B_4C (natural enrichment) sintered pellets located symmetrically within the outer core (white rods in Figure 1).

3. CROCUS calculation schemes

Two main calculation schemes are considered in this paper. The first one is a Monte Carlo approach, the other one is a deterministic approach using the so-called multi-step methodology.

3.1 Monte Carlo Approach

In the present work, the Monte Carlo codes MCNP5 [1] and SERPENT (v1.1.19) [2] are used, MCNP5 being the reference solution. Both Monte Carlo solutions are using the ENDF/B-VII.0 cross-section library (using the ACELIB library coming with the respective code distribution). Six other libraries are considered also with SERPENT in Section 5.1: JEF-2.2, JEFF-3.1, JEFF-3.1.1, and the ENDF/B-VI.8 libraries, ACE formatted libraries provided with the SERPENT distribution and JEFF-3.2, also an ACE formatted library downloaded from the JEFF website. The cross-section data are generated at room temperature (293 K) with NJOY-99.161.

The MCNP5 and SERPENT CROCUS models were developed based on the specifications of [3]. The MCNP5 model was developed in-house while the SERPENT model is provided by the VTT Technical Research Center of Finland.

Unless otherwise specified, the Monte Carlo solutions are obtained using 800 cycles of 10^5 neutrons each. The first 100 cycles are discarded. The resulting relative standard deviations on k_{eff} are around 15 pcm.

3.2 Deterministic Approach

Lattice physics applications with Monte Carlo approaches are often considered impractical because of high computational costs. Typically other lattice physics codes are used (e.g. CASMO[4] or SCALE[5]) to process the homogenized group constants needed for a simulator. However due to the unique CROCUS design, the use of Monte Carlo code like SERPENT became highly advantageous for nuclear data library generation. SERPENT's flexibility with modeling geometries allows defining non-regular regions where homogenization occurs as seen in Section 4.1. Such use of SERPENT has already been made for Sodium Fast Reactor analysis as reported in [6]. The use of SERPENT as a lattice code to generate the nuclear data library needed by the core simulator in the multi-step approach allows insuring consistency in the nuclear data when comparing PARCS results to SERPENT.

The core simulator considered in this work is PARCS [7]. PARCS is a neutronic code developed at Purdue University. It is a 3D reactor core simulator, which solves the steady-state and time-dependent, multi-group neutron diffusion and low order transport (SP3) equations.

The various calculation paths considered in this work are illustrated in Figure 2. The nuclear data library for PARCS is generated with SERPENT. Two main approaches are available to

provide PARCS with macroscopic cross-sections. One involves the specification of reference cross-sections and derivatives by hand in the input deck. The second one involves PMAXS files generated by the GenPMAXS code [8] which is capable of reading a few different lattice codes' output. SERPENT does not produce PMAXS files by default. However, a set of scripts written in Python have been developed at MIT to run SERPENT as a lattice code with branch calculations and to produce a PMAXS library for use in PARCS. Those scripts, commonly called SerpentXS [9], have been provided by MIT and are used to generate the PMAXS files from the SERPENT outputs.

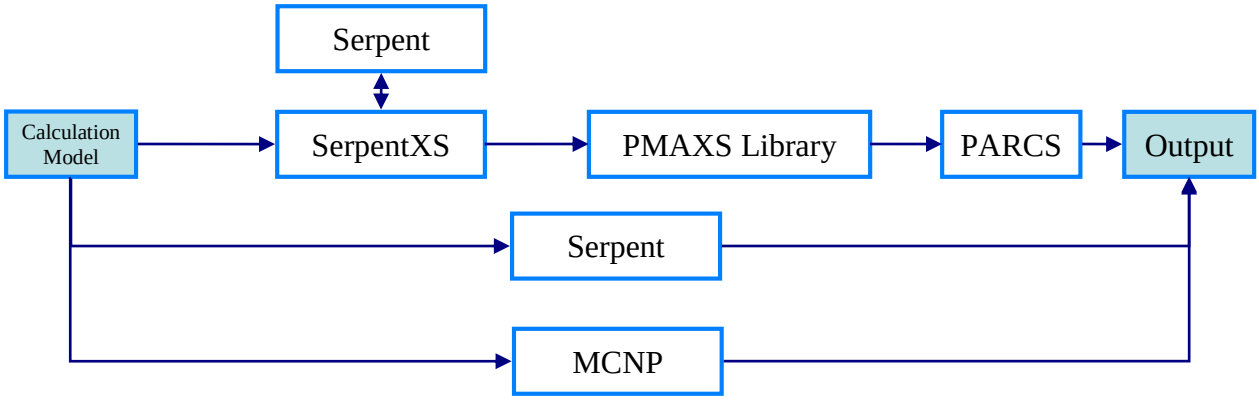


Figure 2 CROCUS calculation schemes

4. CROCUS PARCS model development

In the present section, the development of the PARCS model for CROCUS is described. It consists of two steps, the definition of the subset of the geometry on which lattice calculations are performed to generate the nuclear data library and the development of a 3D CROCUS model in PARCS.

4.1 Nuclear data preparation

In the first step of the multi-step approach, a lattice code is used to generate a nuclear data library by spatial homogenization and energy condensation. Spatial homogenization for large-scale power reactors is done at the assembly level with specular boundary conditions, effectively simulating an infinite lattice of identical assemblies. The homogenization procedure assumes that local physical properties within each region where the homogenization is done depend mostly on physical properties and thermal hydraulic conditions inside the assembly rather than on the assembly's global position in the core. This assumption is acceptable in normal practice for large-scale power reactors, but encounters some difficulty when applied to CROCUS and other small reactors like it.

In CROCUS, the diameter of the active element of the core is 58.34 cm and the total reactor diameter is 100 cm with the water reflector included. The assumption of insular macroscopic cross-sections in each homogenization region is not as solid for this reactor as each region,

including the reflector, will be more closely coupled to its neighbors, affecting the regions' fluxes, and thus the macroscopic cross-sections.

Complications also arise due to the two nested lattices with distinct pitches as shown in Figure 1. The pitch of the inner UO_2 lattice and the outer U-metal lattice are shown in Figure 3. They are incongruous, creating a water gap at their interface. Due to the small size of the core, this heterogeneity has an impact on the core's neutron flux spectrum which needs to be taken into account. The incongruity also means that the core has no definite and symmetrical subunits like an assembly into which it can be subdivided for cross-section homogenization.

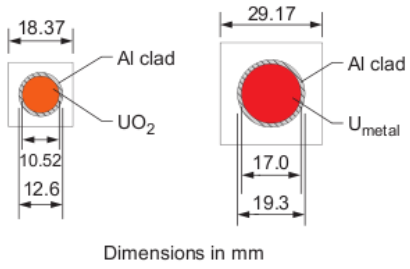
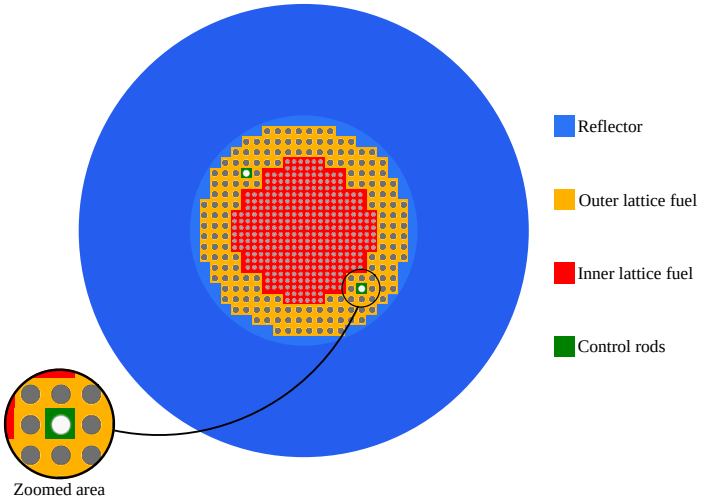


Figure 3 Pitch Comparison of inner (left) and outer (right) lattices of CROCUS [3]

In this work, the 2 energy group macroscopic cross-section library for PARCS is generated as follows. The full core geometry is modeled in 3D and the local neutron flux distribution, accounting for neutron leakage, is used for spatial homogenization and energy condensation. The outer and inner lattices, the reflector, and the control rods are defined as separate regions for which distinct sets of macroscopic cross-sections are obtained by SERPENT. Figure 5 shows how each region is defined. The water gap between the inner and outer lattices is included in the inner lattice homogenization region.

The cross-sections for the reflector are generated by homogenization of the water region outside the outer-fuel lattice. For control rods cross-sections homogenization, another homogenization region is defined, containing only the control rod's unit cell as shown in Figure 4.



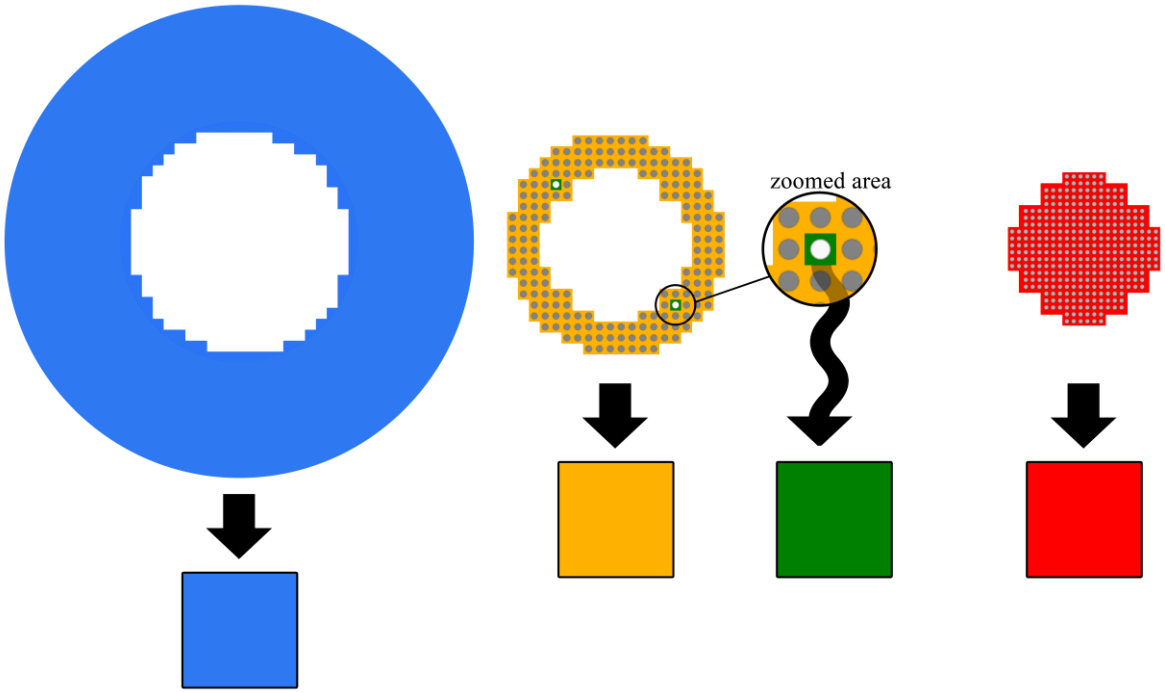


Figure 4 Homogenization regions for Full Core scheme - Each color represents a set of macroscopic cross-sections

4.2 PARCS model

The second step is to develop a model of the CROCUS core in PARCS. Due to its complex design, the radial node size in PARCS is taken to be the pitch of the outer fuel lattice, about 2.9cm which is much smaller than the usual 20cm used in Light Water Reactors. The radial-node geometry of the PARCS model of CROCUS is developed as illustrated in Figure 5. Because the nodes in the PARCS grid must be symmetrical, the size of the nodes of the outer and inner lattices must be the same. The outer-lattice unit cell is used because it has a grid size that can divide the core while maintaining its total area. In addition because modeling control rod withdrawals is essential to the project, the size of the nodes where the two control rods are located, i.e. in the outer fuel zone, cannot be changed. The disadvantage of this method is that it ignores the water gap between the lattices, and the nodal power in the inner lattice does not correspond to the relative power generated by each fuel rod of the inner lattice since the inner lattice is not concurrent with the nodalization.

Axially the active fuel region is divided into 25 nodes, each being 3.8088 cm in length, for a total length of 95.22 cm. 95.22 cm is the reactor's water level set in SERPENT and MCNP5. The real fuel rods are 100 cm in length, meaning that in the PARCS model, the 4.78% of unmoderated fuel is neglected. The baseplate below the fuel rods and the water beneath the core were also included as several axial reflector nodes for a total depth below the fuel of 47 cm. These axial-reflector nodes use the same cross-section sets as the radial-reflector nodes, effectively neglecting the structure below the core containing the start-up neutron source. This

approximation is expected negligible for the PARCS solution, compared to the other approximations made so far (homogenization of the inter-lattice water gap, etc…). No reflector nodes are included above the water level because this area is only air and a small portion of Al and unmoderated fissile material, which would only reflect a small fraction of neutrons. The control rods are defined using the specific option and description present in PARCS, so that they could be removed in steps of 0.5 cm, amounting to 200 steps overall in the model.

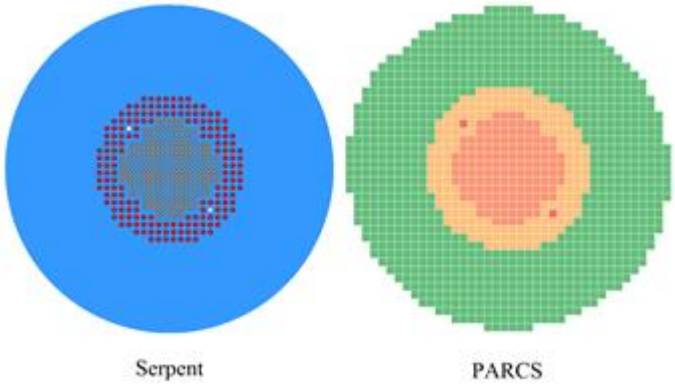


Figure 5 Comparison of SERPENT and PARCS CROCUS models

Due to its small node size, the PARCS solution is effectively a pin-by-pin solution of the CROCUS reactor, where the concept of pin-by-pin is defined in [10]. Consequently, the usual Assembly Discontinuity Factors are not accurate for our purpose and will not be used in this work.

5. CROCUS PARCS model verification

In the present section, the PARCS model described above is compared to the Monte Carlo solutions in terms of k_{eff} and control rod worth. The differences in terms of k_{eff} are expressed in pcm with respect to the MCNP5 solution, using Eq (1):

$$\frac{\Delta k}{k} = \frac{k - k_{MCNP5}}{k_{MCNP5}} x10^5 \quad (1)$$

5.1 K_{eff} comparison

The k_{eff} results predicted by both Monte Carlo codes and PARCS are shown in Table 1.

Table 1 k_{eff} comparison for between SERPENT and PARCS

Code	k_{eff}	Stoch. Unc. [pcm]	Δk/k [pcm]
MCNP5	1.00202	5	--
SERPENT	1.00189	5	-13
PARCS	0.99793	--	-408

The SERPENT and MCNP5 models agree well with each other, the k_{eff} predicted by SERPENT being within three standard deviations of that of MCNP5. However, both Monte Carlo models lead to k_{eff} greater than unity for a critical configuration, the over prediction being about 200 pcm. The PARCS k_{eff} is underpredicted by about 400 pcm with respect to MCNP5 indicating a bias, which is due to the multi-step approach. It is however unclear at this point how significant are those 400 pcm.

Table 2 Impact of nuclear data libraries on k_{eff} prediction from SERPENT

Library	k_{eff}	Stoch. Unc. [pcm]	Δk/k [pcm]
JEFF-3.2	1.00305	15	128
JEFF-3.1.1	1.00191	15	14
JEFF-3.1	1.00131	16	-46
ENDF/B-VI.8	0.99636	16	-541
JEF-2.2	0.99878	16	-299

In order to explain the observed bias (200 pcm) of the Monte Carlo solution with respect to the measured critical water level of CROCUS, other nuclear data libraries than ENDF/B-VII.0 are considered. SERPENT is run with the five additional nuclear data libraries mentioned in Section 3.1 and the results are shown in Table 2. All the relatively new libraries (JEFF-3.1 and higher) lead to an overprediction of k_{eff} whereas the older nuclear data libraries underpredict k_{eff} by about the same amount. This suggests than the observed bias may be coming from nuclear data library used by the Monte Carlo codes and not from an error in the material composition or geometry description.

In order to confirm this hypothesis, the propagation of nuclear data uncertainty in the SERPENT calculation is investigated in the next section.

5.2 K_{eff} uncertainty quantification

The propagation of uncertainty due to the nuclear data in the SERPENT calculations is investigated by doing the uncertainty quantification (UQ) of k_{eff} predicted by SERPENT. The idea is to verify that the deviation from criticality predicted by MCNP5 and SERPENT can be explained by the uncertainty in the nuclear data. Previous studies [11] have shown that such uncertainties account for 500pcm for light water systems. The conventional first-order uncertainty quantification as described in [11] is used and summarized here for completeness.

Consider input, x, and output, y, with nominal values x_0 and y_0. The cornerstone of local, first-order UQ methods is the capability to calculate sensitivity coefficients,

$$S \equiv \left.\frac{\partial y}{\partial x}\right|_{x=x_0} \frac{x_0}{y_0}, \qquad (2)$$

Using the calculated sensitivity coefficients in UQ simply requires the classic first-order uncertainty propagation formula, shown below

$$R = S^T \, V_X \, S, \tag{3}$$

with *R* being the relative standard deviation of the considered output, k_{eff} in this work, in terms of the *relative* variance/covariance matrix (VCM) of the inputs V_X and the sensitivity coefficients, *S*.

Recent developments in MC code allow the use of iterated fission probability (IFP) technique to compute the adjoint flux and consequently the sensitivity coefficients. The IFP method has been implemented in SERPENT [12] to compute the sensitivity coefficients. Due to the peculiarity of the IFP, the Monte Carlo calculations are performed using 500,000 cycles of 2,000 neutrons[†], amongst them 100 are discarded.

The input VCM needed in Eq (3) is the SCALE6 VCM library [13], which contains over 401 materials from a variety of sources, including evaluations from ENDF/B-VII, ENDF/B-VI, JENDL-3.1, plus 300 approximate VCMs such that all remotely relevant nuclides have uncertainty data. In the present work, however, only uncertainty due to U-235, U-238, O-16, H-1 and Al-27 cross-sections, i.e. the main isotopes present in the model, are taken into account.

The results of the UQ are shown in Table 3.

As expected, most of the k_{eff} uncertainty is coming from the capture in U-238, the average number of neutron created by U-235 fission and the inelastic scattering in U-238. As expected, those results are consistent in terms of magnitude and major contributors (isotope reaction pair) of the uncertainty, with respect to the LWR pin-cells' analysis of [11] giving confidence that the first order UQ methodology used in this work leads to reasonable results. The analysis of the sensitivity coefficients predicted from SERPENT also shows some interesting trends. Although its sensitivity to k_{eff} is high, the uncertainty due to U-235 fission is small because the U-235 fission cross-section is very well known, i.e. has a very small input uncertainty. It is the opposite for the U-238 inelastic scattering for which k_{eff} has a small sensitivity coefficient. However, because of its high uncertainty, this reaction is one of the main contributors to the overall k_{eff} uncertainty.

Table 3 SA and UQ on CROCUS k_{eff} with SERPENT

Rel. Std		0.573%	
Main Contributors	**Nuc. Reac.**	**Sensitivity Coefficient**	**Rel. Std.**
	U-238 σ_c	-0.245	0.36%
	U-235 ν	0.933	0.28%
	U-238 $\sigma_{s,\,inel}$	0.013	0.19%
	U-235 σ_c	-0.097	0.17%
	U-235 σ_f	0.409	0.16%

[†] The small number of neutrons per cycle and high number of cycles do not introduce a bias in the MC estimation of k_{eff} in this case.

The other major finding of the UQ on CROCUS k_{eff} is that the uncertainty due to nuclear data, 0.573% in relative terms or about 600 pcm in absolute terms, covers the deviations of k_{eff} predicted by both MCNP5 and SERPENT from unity. It means that no obvious modeling errors (geometry, material composition, simplifications) are present in the Monte Carlo models considered. Finally, the UQ results also show that the discrepancies between PARCS and the Monte Carlo solutions in terms of k_{eff} as shown in Table 1 are acceptable. It should be noted also that no uncertainty for the so-called technological parameters (critical height, coolant temperature, lattice pitch, fuel pin diameters) is taken into account in this study.

5.3 Control rod worth comparison

The last piece of work for the code-to-code comparison is to check the prediction of control rod worth. The change in k_{eff} with change in control rod position is compared first between the SERPENT and MCNP5 models to verify the accuracy of the SERPENT model's geometry and material input, and then between SERPENT and PARCS. Accurate modeling of the control rods is especially important in this work because they are the means by which reactivity is inserted in the core in transient analyses with PARCS.

Table 4 Control rod worth comparisons

Control Rod Model	Reactivity Worth (Δρ)
MCNP5	174 ± 7 pcm
SERPENT	169 ± 6 pcm
PARCS	136 pcm

The control rods worths in pcm predicted by each code are shown in Table 4. MCNP5 and SERPENT agree within one standard deviation of their stochastic uncertainty and are very close to the experimental rod worth of 165 +/- 1 pcm [14]. However, the result is less satisfying with PARCS which strongly underpredicts the rod worth, i.e. 140 pcm compared to 170 pcm for the Monte Carlo solutions. A potential explanation for such phenomena is related to the definition of the homogenization regions in SERPENT. The influence of the presence of the control rod on the surrounding fuel rods is not taken into account in the homogenization process because the homogenization region of the control rod is limited to the control rod itself and not the surrounding fuel rods as shown in Figure 2. As a consequence, the local spectral hardening and consequently decrease of reaction rates of the nearby fuel due to the presence of the control rod cannot be properly captured leading to an underprediction of the rod worth.

Further improvements of the control rod modeling technique will address this issue by increasing the size of the region for control rod cross-section homogenization.

6. Conclusions

The present work described the successful development and preliminary verification of a 3D nodal simulator PARCS model of the CROCUS reactor. The set of macroscopic cross-sections needed by PARCS is generated by the Monte Carlo code SERPENT using the full core 3D flux solution for spatial homogenization and energy condensation.

The verification of the PARCS model has been made based on k_{eff} and the control rod worth as quantities of interest. The reference solutions are provided by whole-core calculations using two Monte Carlo codes, MCNP5 and SERPENT. It was shown that both SERPENT and MCNP5 agree within their stochastic uncertainty. PARCS k_{eff} predictions are within 400 pcm of the SERPENT results. It is found to be an acceptable agreement since the uncertainty in the prediction of k_{eff} due to uncertainty in the continuous energy cross-sections is shown to be about 600 pcm. Such uncertainty also covers the deviation from unity of the k_{eff} prediction by MCNP5 and SERPENT for the critical CROCUS configuration.

Future work will aim at comparing the local pinpower prediction of PARCS and the Monte Carlo solutions. Additional homogenization schemes will also be investigated to improve the relatively inaccurate control rods worth prediction of PARCS. The validation of the PARCS models against experimental measurements is also planned in the near future.

7. References

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