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SERPENT-PATHS Coupling Program: Calculations on the RBWR

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Abstract - *The development of new reactors such as the Resource-Renewable Boiling Water Reactor (RBWR) requires an innovative advanced design method. Current core design methodologies for nuclear reactors involve the use of deterministic codes that rely on nodal diffusion methods with few group cross sections that are generated by lattice physics codes. The improvement of the reactor behavior analysis is today concentrated on the implementation of high fidelity multi-physics codes that gathers growing interest with the availability of high performance computing facilities. Coupled multi-physics codes are needed to describe the complex operations happening within reactor cores. The traditional approach to reactor analysis couples a neutronics deterministic code and a thermal-hydraulics code. This method relies on a multi-stage calculation scheme divided in two steps combining spatial homogenization and core simulation. An alternative to this approach is based on a Monte Carlo neutronics code coupled to thermal-hydraulics codes. This paper presents the development of a new method – McCI - for coupled neutronics and thermal-hydraulics codes. The Monte Carlo Coupling Interface (McCI) couples the Monte Carlo neutronics code SERPENT and the U.S. NRC thermal-hydraulics code PATHS. The approach has been implemented within the context of the safety survey of the RBWR and results on the functioning characteristics are presented. The approach has provided convincing results for a single assembly of the RBWR. The comparison between SERPENT-PATHS and PARCS-PATH has underlined significant differences. As SERPENT-PATHS coupling method is the more accurate model, these results demonstrate that the cross sections used in PARCS induced an inaccurate representation of the RBWR behavior.*

I. INTRODUCTION

Core design methodologies for nuclear reactors involve the use of deterministic codes that rely on nodal diffusion methods with few group cross sections that are generated by lattice physics codes[1]. This two-step calculation in deterministic analysis provides fast and accurate solutions for standard LWRs. However, it is not certain that these standard methods are applicable to new reactor designs, such as Resource-Renewable Boiling Water Reactor (RBWR). In order to verify the applicability of two-step methods for new reactor designs, benchmark problems using higher order methods on smaller scale models are needed. The improvement of the reactor behavior analysis is today concentrated on the implementation of high fidelity multi-physics codes - based on stochastic approach – which gathers growing interest with the availability of high performance computing facilities. With the development of dynamic Monte Carlo and the development of coupled-steady state Monte Carlo calculations, the road has been paved to perform transient analysis of high power reactors using stochastic methods[2]. In this way, it is possible to take into account the thermal-hydraulic feedback, while the neutron transport is modeled in full detail.

Coupled multi-physics solutions are needed to describe the complex operations taking place inside the reactor core. The traditional approach to reactor analysis couples a neutronics deterministic code and a thermal-hydraulics code[3]. This method relies on a multi-stage calculation scheme divided in two steps: 1) Spatial homogenization, where the interaction physics at the fuel assembly level is condensed into a set of assembly-specific multi-group constants, and 2) Core simulation, where the full-scale neutronics solution obtained using diffusion theory or other simplified transport method is iteratively coupled to thermal hydraulics.

However, a more accurate approach is available, making use of a Monte Carlo neutronics code such as SERPENT[3] or MCNP[4], coupled to thermal-hydraulics codes. This second method provides reference data for new reactors and benchmarks that are required to verify the consistency of lower order methods.

Many other coupled Monte Carlo neutronics/thermal-hydraulics systems were developed to solve various problems. Seker et al. (2007) used coupled MCNP5/STAR-CD to simulate a 3-D by 3 array of PWR fuel pins[5].

The RBWR is part of the Advanced Boiling Water Reactors (ABWR) series developed by GE Hitachi and Toshiba. This reactor possesses the unique feature to burn transuranic nuclides produced by conventional reactors. This characteristic gives access to long-term energy supply, while greatly reducing the negative environmental impact of transuranic elements, which are becoming long-lived radioactive wastes[6]. These materials called transuranics are heavier than the uranium used for fuel rods and originate from spent Light Water Reactor (LWR) fuel. The classic

LWR do not burn completely transuranics because water slows down neutrons while transuranics are more efficiently burned when hit by fast neutrons.

The optimization of the RBWR requires an advanced analysis in order to assess the various processes in the classical safety surveys. In order to achieve this objective, the modeling approach has to be improved by combining a Monte Carlo based neutronics code with a thermal-hydraulics model. This selected approach is based on SERPENT[3] and PATHS (PARCS Advanced Thermal Hydraulic Solver)[7] codes.

This paper presents the development of a new method for coupled neutronics and thermal-hydraulics codes. The Monte Carlo Coupling Interface (McCI) couples the Monte Carlo neutronics code SERPENT and the U.S. NRC thermal-hydraulics code PATHS. The approach has been implemented within the context of the safety survey of the RBWR and results on the functioning characteristics are presented.

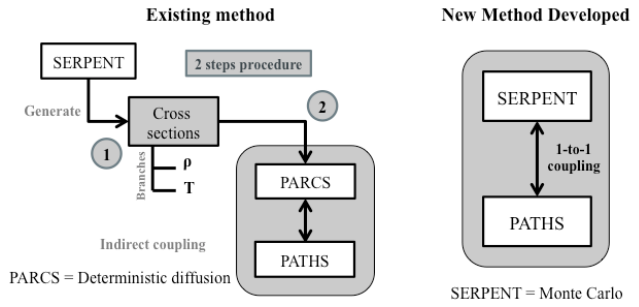

Fig. 1. Diagram showing the old and new coupling methods.

II. THE McCI COUPLING METHOD

In order to obtain higher accuracy in reactor processes modeling, coupling a Monte Carlo neutronics code with a thermal hydraulic model represents a meaningful approach especially for new complex reactor designs such as the RBWR. The selected approach for McCI (Monte Carlo Coupling Interface) is based on SERPENT[3] version 2.1.22 and the PATHS v1.02 module[8] of PARCS[7].

1. SERPENT: a Monte Carlo neutronics code

SERPENT is a three-dimensional continuous-energy Monte Carlo reactor physics burnup calculation code[3]. This lattice physics calculation code allows high fidelity simulations of the behavior of a reactor core. SERPENT uses a universe-based combinatorial solid geometry (CSG) model, which allows the description of practically any two- or three-dimensional fuel or reactor configuration. The geometry consists of material cells, defined by elementary quadratic and derived macrobody surface types. The Monte Carlo simulation can be run in k-eigenvalue criticality source or external source mode. Neutron transport is based on a combination of conventional surface-to-surface ray-tracing and the Woodcock delta-tracking method[9]. SERPENT reads continuous-energy cross-sections from ACE format data libraries. The interaction physics is based on classical collision kinematics, ENDF reaction laws and probability table sampling in the unresolved resonance region. Improved treatment for the free-gas scattering kernel near resonances is also available, based on the DBRC Doppler-broadening rejection correction method (Becker, 2009)[10]. A built-in Doppler-broadening preprocessor routine allows the conversion of ACE format cross sections into a higher temperature. This capability results in a more accurate description of the interaction physics in temperature-sensitive applications, as the data in the cross section libraries is available only in 300K intervals. In addition to the pre-processor routine, SERPENT 2 has the option to adjust nuclide temperatures on-the-fly. User-defined tallies can be set up for calculating various integral reaction rates. The spatial integration domain can be defined by a combination of cells, universes, lattices and materials, or using a three-dimensional super-imposed mesh. The number and structure of detector energy bins is unrestricted. Various response functions are available for the calculation, including material-wise macroscopic and isotopic microscopic cross sections and ACE format dosimetry data. SERPENT 2 calculates adjoint-weighted point kinetics parameters and effective delayed neutron fractions using the iterated fission probability (IFP) method (Leppänen, 2014b)[11], relying on an implementation similar to that in MCNP5 (Kiedrowski, 2011)[12]. SERPENT 2 has high computational requirements, which can increase significantly with large models, such as a full core nuclear reactor model.

2. PARCS: a deterministic neutronics code

The Purdue Advanced Reactor Core Simulator (PARCS)[7] is a three-dimensional reactor core simulator that solves the steady-state and time-dependent neutron diffusion or SP3 transport equations to predict the dynamic response of the reactor to reactivity perturbations such as control rod movements, boron concentration or changes in the temperature/fluid conditions in the reactor core. The code is applicable to both PWR (Pressurized Water Reactor) and BWR cores loaded with either rectangular or hexagonal fuel assemblies. PARCS integrates a thermal hydraulic module – PATHS - to achieve a precise representation for most of the BWR processes. The PATHS[8] code is developed to solve the steady state thermal-hydraulic condition of a BWR. The module provides thermal hydraulic feedback for state and depletion calculations. The tight coupling of the thermal hydraulic and neutronics fields for a BWR makes it essential to accurately model the density and temperature distribution in the reactor. PATHS has the ability to model parallel flow channels and distribute the core flow in the channels such that the pressure drop across the core is uniform in all

channels. PATHS can also be executed as a standalone thermal hydraulic solver with a specified power distribution. PATHS code utilizes an approach relying on a four-equation drift flux model with simplified equations and solution algorithms that considerably reduce the runtime while maintaining sufficient accuracy of the solution for steady-state depletion analysis. In particular, the simultaneous solution of the mass and momentum equations automatically calculates the proper flow distribution to give an equal pressure drop in all channels, without the need for time-consuming iteration between velocity and pressure. The efficient runtime in PATHS is particularly advantageous for applications requiring the use of a unique "one to one mapping" of a thermal hydraulic channel for each fuel assembly and repetitive steady-state core thermal hydraulic solutions during core burnup and equilibrium cycle search calculations.

3. McCI key steps

The key steps of the McCI coupling interface are the following:

- SERPENT neutronics code runs on an initial set case and returns the neutron flux and power distribution;
- The power distribution is extracted form SERPENT outputs and used to generate the new PATHS input file using the normalized power shape;
- The thermal-hydraulics code PATHS solves the temperature and fluid conditions in the reactor;
- The temperature and fluid feedback from PATHS output is then passed back to SERPENT. The fuel temperature and water density is updated in the SERPENT input file;
- The program iterates at this point, running alternatively SERPENT and PATHS, until the coupled neutron and temperature/fluid fields converge. At each iteration, the power distribution and the temperature/fluid conditions are updated using the feedback of each code.

The McCI coupling interface between SERPENT and PATHS has been written in Python 3.5.1[13] and its goal is to run both coupled codes until the given convergence criterion is respected. The criterion is defined using the second norm – or infinite norm - of the relative difference between the current and the previous iteration for 3 variables (power, water density and fuel temperature).

At the current stage, McCI has been designed for a single assembly from the RBWR. This version could be modified to fit other configurations as for the full core model of the RBWR. McCI requires three files to be executed:

- The RBWR SERPENT input file which is used as initial condition;
- The RBWR PATHS input file which is only used as a template for future iterations;
- McCI input file which allows the user to easily define parameters such as the convergence criterion, the norm used for convergence, ...

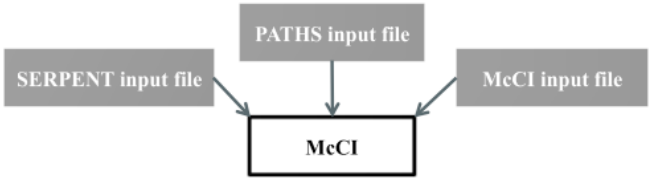

Fig. 2. Diagram of the input files needed to run McCI.

As McCI runs several iterations, the following steps are repeated for each iteration:

- The initial Serpent run is performed with the initial condition file;
- The axial power distribution is extracted from its output file;
- This power shape is normalized and used to create a new PATHS input file based on the template of the PATHS input file. In case of a previous iteration, the second – or infinite – norm of the relative difference between the power of the current iteration and the previous one is compared to the convergence criterion.
- Once PATHS new input file is established, PATHS code is run;
- Fuel temperature and water density are extracted from the output files. These data are used to create a new input file for SERPENT. In case of a previous iteration, the second – or infinite – norm of the relative difference between the fuel temperature and water density of the current iteration and the previous one is compared to the convergence criterion;
- McCI iterates and SERPENT runs the input file previously written for all the next iterations;
- If all three variables - power, water density and fuel temperature - respect the convergence criterion in the same iteration, the program stops and results are available. If the criterion is not satisfied, the program loops and a new iteration starts by running the new SERPENT input file.

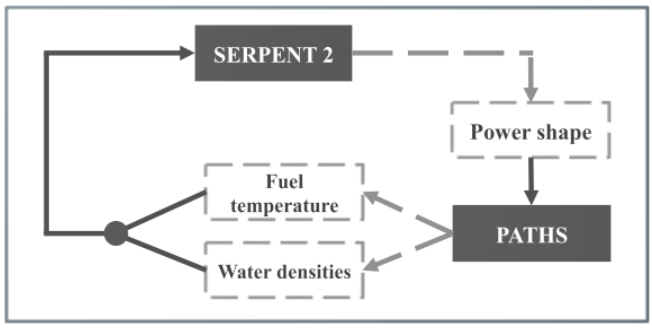

Fig. 3. Functioning diagram of McCI.

4. Application case

McCI has been implemented and applied on a model of a single assembly of the RBWR. The RBWR designs deserve to be considered among the candidates for next-generation reactors[14]. They provide a possibility for more efficient use of uranium resources - compared to Light Water Reactors (LWR) - and for the near-complete elimination of the long-lived transuranic waste. Since these designs use the well-established light water technology, their commercialization is likely to require a significantly shorter time and smaller investment in research and demonstration than their sodium-cooled alternatives. Two cores whose fuel bundles are compatible with each other, but have different purposes, have been proposed so far; they are the break-even reactor (RBWR-AC) and the TRU burner (RBWR-TB). The RBWR is capable of making the transition between the RBWR-AC and the RBWR-TB by changing fuel bundles.

McCI has been implemented on a modified version of the RBWR-TB core, the RBWR-TB2. The RBWR-TB2 is designed to be able to burn TRUs from LWR spent fuels, while the RBWR-TB is designed as a burner for the TRUs from the RBWR-TB itself.

The geometry of a RBWR single assembly is divided in thirty successive layers:

- 2 Lower reflector layers;
- 8 Lower fissile layers;
- 8 Internal blanket layers
- 8 Upper fissile layers;
- 2 Upper blanket layers;
- 2 Upper reflector layers.

The axial power distribution of the fissile and blanket regions has been calculated and analyzed. As demonstrated later, it has been used to verify the consistency of the method using the power output and normalizing it to one over the total height.

The unique design of the core has presented several challenges for computer codes used to analyze the core since the axial fuel design consists of several axially alternating blanket and fissile fuel regions in order to increase breeding of plutonium in the blanket[15]. This creates a severe double peaked power distribution and axial heterogeneities that are not typical of light water reactors (LWRs) and poses challenges to the conventional methods used for LWR design and analysis. This situation underlines the interest to develop a high-fidelity multi-physics method.

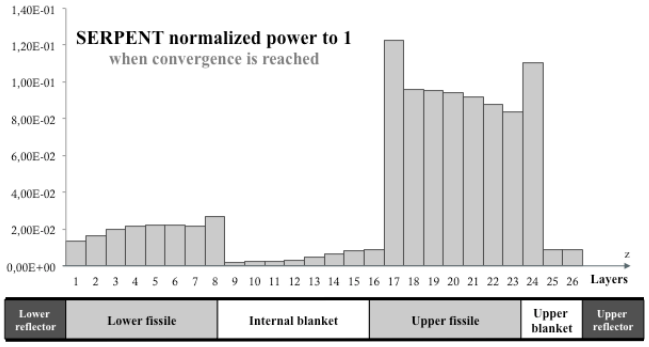

Fig. 4. Normalized axial power distribution of the RBWR.

5. Fuel temperature implementation

The fuel temperature is extracted from PATHS output for each axial layer and used for the creation of the new SERPENT input file. The temperature can be included within the boundaries of the 300K cross-sections intervals. Two procedures can then be implemented to match the PATHS temperature constraints.

The first procedure is to update the fuel temperature using the *tmp* command in SERPENT that initiates the Doppler broadening routine to modify the nuclides temperature[3]. This method is the most accurate one although this command significantly increases the computing time and makes it prohibitive for larger models.

```
mat fuel   -10.45700 tmp 1000
92235.09c   -0.03173
92238.09c   -0.84977
 8016.09c   -0.11850
```

Fig. 5. Tmp SERPENT command example.

The second solution is to implement a weighting method between cross-sections. The chosen protocol is the following: if 600K and 900K cross-sections are available and that the fuel temperature given by PATHS is 650K, five sixth (900-650)/300=5/6 of the initial concentration is attributed to the 600K cross-section and one sixth (650-600)/300=1/6 is attributed to the 900K.

The accuracy of this last protocol using a barycenter method has been checked by running a test case with both methods. Very similar results were obtained regarding the power shape and the eigenvalue, which ensures the accuracy

of the method. The maximum relative difference between both methods is only 0.98% and the K_{eff} obtained were equal.

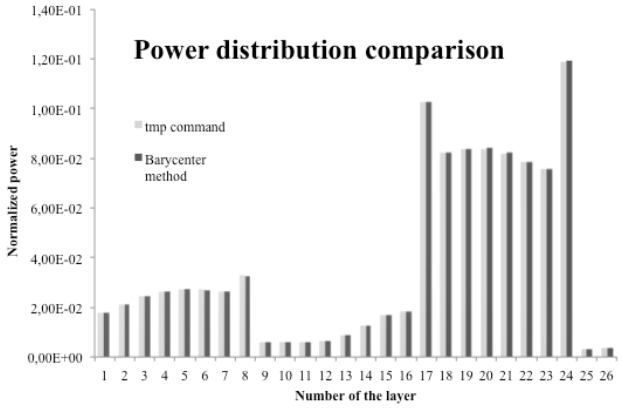

Fig. 5. Comparison of the two temperature implementation methods.

The water density, extracted from the PATHS output file, is used in the materials definition in the SERPENT input file generated for the next iteration. The axial power distribution is extracted from the SERPENT output file and used as an input for PATHS run.

6. Convergence norms available

Two norms are available for the convergence method of the McCI procedure: the infinite and the 2-norm. Both are calculated on the total height of the reactor:

- Infinite norm: the relative difference between the current iteration and the previous one is determined for each layer of the model. The maximum value is compared to the corresponding convergence criterion.

$$\frac{|X_i^{CurrentIteration} - X_i^{PreviousIteration}|}{X_i^{CurrentIteration}} = Rel.Diff \qquad (1)$$

Infinite norm calculation.

- 2-norm: the relative difference between the current iteration and the previous one is determined using the 2-norm on all layers of the model. The value of *errsquare* is then compared to the convergence criterion of the corresponding variable.

$$err = |X_i^{CurrentIteration} - X_i^{PreviousIteration}| \qquad (2)$$

Intermediate variable calculation.

$$err2nd = \sum_{i=0}^{30} err^2 \qquad (3)$$

Intermediate variable calculation.

$$errsub = \sum_{i=0}^{30} X_i^{CurrentIteration}.X_i^{PreviousIteration} \qquad (4)$$

Intermediate variable calculation.

$$errsquare = \sqrt{\frac{err2nd}{abs(errsub)}} \qquad (5)$$

2-norm final calculation.

7. Under-relaxation

For each iteration, power distribution, fuel temperature and water density are calculated based on the previous iteration results. The following under-relaxation formula is used for under-relaxation, X_i being the variable at the ith iteration:

$$X^i = (1 - C_u).X^{i-1} + C_u.X^i \qquad (6)$$

Under relaxed variable calculation.

A source file is being used for the SERPENT run in the McCI protocol. This procedure allows a better accuracy and reduces the number of iterations required before reaching convergence.

III. RESULTS

As SERPENT is a stochastic simulation code, SERPENT-PATHS coupling is a one to one coupling method, meaning that the results obtained are very close to the actual behavior of the reactor. This higher order method provided a useful and accurate benchmark for PARCS-PATHS method. The results obtained with the new SERPENT-PATHS coupling method are compared with the outputs of the existing PARCS-PATHS coupling method applied on a RBWR single assembly. The PARCS v32 has been used for these tests.

The SERPENT-PATHS program was run several times to optimize the convergence parameters including the convergence criteria, the under-relaxation coefficient and the convergence method. Once the optimal parameters were found, a reference case was established in order to compare it with the deterministic PARCS-PATHS coupling. The main parameters defining the simulation were the following ones:

- Convergence criteria: 10^{-3} for all three variables studied (power, fuel temperature and water density);
- Under-relaxation coefficient: 0.3 for all three variables;
- Convergence method: 2-norm.

The simulation converged after 13 iterations. The evolution of the relative difference between the current iteration and the previous one, for each factor and the convergence criterion to attain, are displayed on Fig. 6.

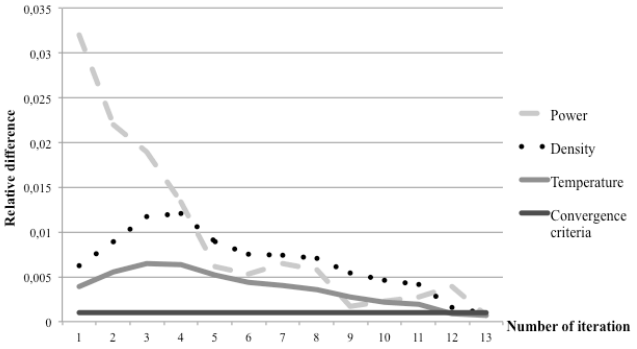

Fig. 6. McCI variables convergence.

Although SERPENT-PATHS results are more accurate, they should be reasonably consistent with PARCS-PATHS coupling regarding the axial power shape and the eigenvalue, once convergence is reached for SERPENT (13^{th} iteration).

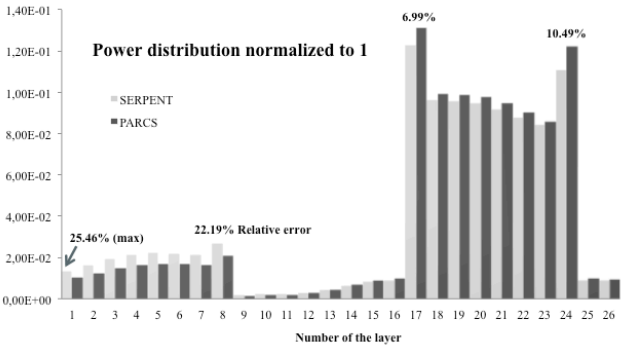

Fig. 7. Normalized power distribution for SERPENT and PARCS.

PARCS-PATHS and SERPENT-PATHS power distributions have a similar global shape but present locally significant differences. The relative error between both methods reaches 25.46%, which is around 6.10^{-3} on a scale of 1. The obtained eigenvalues have a 350 pcm (per cent mille) difference:

- SERPENT-PATHS: K_{eff} =1.05892
- PARCS- PATHS: K_{eff}=1.06242

Several tests were run to understand the origins of the discrepancies observed. The cross section used in the deterministic code have been checked through 4 tests:

- T1: Using SERPENT data after convergence to generate cross sections for PARCS to recreate the solution;
- T2: Running PARCS in restart mode to recreate the conditions of the last iteration;
- T3: Running PARCS in standalone mode to compare the eigenvalue for the initial case;
- T4: Simulation of the initial case with PARCS in restart mode.

Regarding the uncertainties in the SERPENT calculation, the following figures were obtained:

- Eigenvalue uncertainty: 0.00023 which is reasonably low.
- The local power uncertainty is always inferior to 0.01 for each layer. Considering it is below 1%, the uncertainty is acceptable.

Test 1: Cross section generation.

The neutronics code PARCS is run with fix cross sections, generated based on the final iteration of McCI. Both power shapes are very close as the maximum relative difference between both models is only 2.5%. There is a 46 pcm difference between the two methods K_{eff}, which is quite low.

- SERPENT-PATHS K_{eff}=1.05892
- PARCS-PATHS K_{eff}=1.05846

SERPENT calculation uncertainties are the same as in the previous case as the same SERPENT results were used (convergence reached).

Test 2: Restart mode for the last iteration.

The neutronics code PARCS is run in restart mode, using the last iteration McCI data (concentration and temperature) to recreate the final conditions before convergence. Both power shapes present a significant difference as the maximum relative difference is 16%. The difference between the K_{eff} of the two methods is important: 541 pcm.

- SERPENT-PATHS K_{eff}= 1.05892
- PARCS- PATHS K_{eff}= 1.06433

SERPENT calculation uncertainties are the same as in the previous case as the same SERPENT results were used.

Test 3: Initial case – PARCS standalone.

PARCS is run in standalone mode using SERPENT generated fix cross sections for the initial case. Results are extracted before the first loop of the McCI. Both power shapes are very close as the maximum relative difference is 3.5%. The two eigenvalues are almost the same with a 6 pcm difference only.

- SERPENT-PATHS K_{eff}= 1.06559
- PARCS-PATHS K_{eff}= 1.06565

For this initial case, the eigenvalue uncertainty in the SERPENT calculation is 0.00024. As in the previous tests, the local power uncertainty is always inferior to 0.01 for each layer. These figures are similar to the one obtained for convergence and are reasonably acceptable.

Test 4: Initial case – PARCS restart mode.

PARCS is run in restart mode to recreate the initial conditions using the data given before the first iteration. There is a noticeable disparity between the power distributions for each method: the relative difference between McCI and PARCS reaches 13%. Both K_{eff} are distant from 283 pcm which is relatively high.

- SERPENT-PATHS K_{eff}= 1.06559
- PARCS-PATHS K_{eff}= 1.06842

SERPENT calculation uncertainties are the same as in test 3 as the same SERPENT results were used (initial configuration).

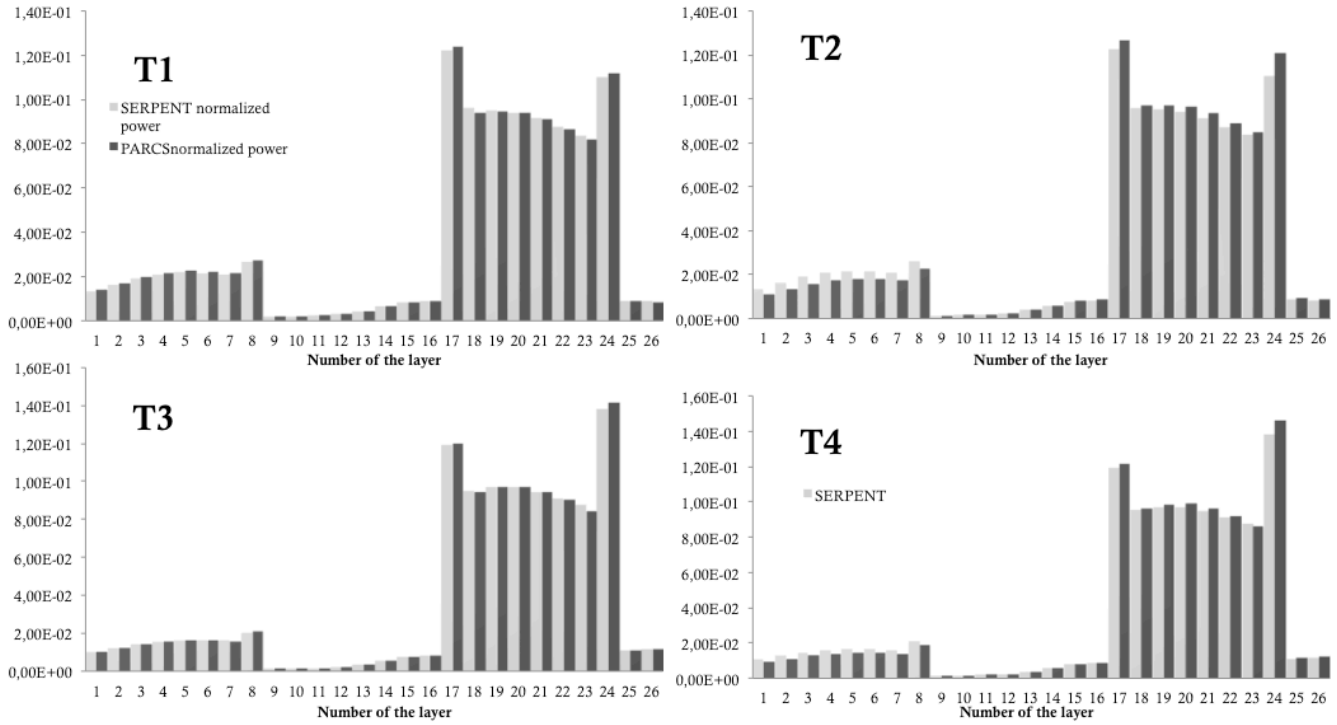

Fig. 8. Normalized power comparison for all four tests.

The tests demonstrate there is a significant difference between the two methods, which seems to be mainly coming from the cross sections. When cross sections generated by SERPENT are used with PARCS, the results obtained are very close to the one from the SERPENT-PATHS coupling (eigenvalue and power shape). Error may be coming from a branch of the cross section that is not taken into account (so far, just temperature and density) or from the fact that the cross section are generated from a burnup case and extracted when the burnup has not started. It may also be due to the unique power shape of the reactor, which is very unusual and hard to handle for deterministic simulation codes.

IV. CONCLUSION

The McCI method allows to couple successfully SERPENT neutronics code with the thermal hydraulic solver PATHS. The approach has provided convincing results for a single assembly of the RBWR. The comparison between SERPENT-PATHS and PARCS-PATH has underlined significant differences. As SERPENT-PATHS coupling method is the most accurate model, these results

demonstrate that the cross sections used in PARCS induced an inaccurate representation of the RBWR behavior.

The current application was limited to a single assembly but work has begun on application to a full core RBWR model. The McCI can be easily used and improvements in the future will include code verification and validation (V&V) and software quality assurance (SQA).

NOMENCLATURE

$X_i^{CurrentIteration}$ = McCI variable (fuel temperature, water density or power) extracted from the current iteration of the program. i indicates the corresponding layer in the model.
$X_i^{PreviousIteration}$ = McCI variable extracted from the previous iteration of the program. i indicates the corresponding layer in the model.
Rel.Diff = relative difference calculated for the infinite norm.
X^i = McCI variable extracted from the ith iteration.
C_u = under-relaxation coefficient.

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