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Macroscopic Cross Section Generation with SCALE 6.2 for the MYRRHA Minimal Critical Core

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Abstract - *The deterministic multi-group code NEWT of the SCALE 6.2 code package is applied for the generation of macroscopic few-group cross sections for use in whole-core calculations of the MYRRHA minimal critical core with the nodal diffusion code PARCS. The available 252-group library from SCALE 6.2 is optimized for light water reactor applications in terms of the weighting spectrum and the energy group structure. Therefore new multi-group libraries optimized for fast reactor applications are applied in this study. At fuel assembly level, the influence of the multi-group library on the multiplication factor is negligible. But the neutron flux spectra obtained with NEWT and the new 302-group libraries show large improvement towards the 252-group LWR library in comparisons with the corresponding reference KENO continuous-energy neutron flux. PARCS calculations of the whole MYRRHA core at four different configurations are compared with reference continuous-energy Serpent Monte Carlo calculations in terms of the multiplication factor, control rod worth and the radial power distribution. It is observed that the influence of the applied multi-group library on the few-group cross section generation with NEWT is negligible. The application of super-cell models for the cross section generation of the outermost fuel assemblies leads to improved agreement regarding the multiplication factor for the uncontrolled core configuration; however, this improvement cannot be observed for other configurations with inserted control rods. Therefore, the deviation on the control rod worth remains important, as it has already been observed in previous studies of the MYRRHA core. The radial power distribution calculated with PARCS shows good agreement with the reference Serpent solutions for all core configurations.*

I. INTRODUCTION

At the SCK-CEN research center in Mol (Belgium), it is planned to build the "Multi-purpose hYbrid Research Reactor for High-tech Applications" (MYRRHA) [1]. This lead-bismuth eutectic (LBE) cooled fast reactor is designed to operate in both critical and sub-critical mode. It serves for the demonstration of the feasibility of accelerator-driven systems and lead-cooled fast reactor concepts. The applications are ranging from burning spent fuel to material irradiation testing.

The widely used SCALE code package [2] offers several modules for reactor physics analysis. Deterministic and Monte Carlo neutron transport codes can be used for criticality and depletion calculations as well as for uncertainty and sensitivity analyses. However, the modules of this code package have so far been especially used and validated for the analysis of light water reactor systems. The performance of the included deterministic neutron transport code NEWT for the generation of homogenized macroscopic few-group cross sections for calculations of a fast reactor system with a nodal diffusion codes needs therefore to be assessed. Since the available multi-group (MG) cross section libraries for the MG solvers are optimized for systems with thermal neutron spectra, new generated MG libraries optimized for fast spectrum systems are applied.

In this present study, macroscopic cross sections are generated for MYRRHA minimal critical core calculations [1] with the nodal diffusion code PARCS [3]. PARCS is a three-dimensional reactor core simulator, developed at the Purdue University, which solves the steady-state and time-dependent multi-group neutron diffusion equation in orthogonal and non-orthogonal geometries. It is coupled with the thermal-hydraulics system code ATHLET [4], developed at GRS, which features were adapted to LBE coolant. This coupling offers the possibility to perform transient calculations in the future. In this study, PARCS was applied as stand-alone code.

The performance of SCALE for macroscopic cross section generation for a LBE-cooled fast reactor core is assessed by comparisons with whole-core calculations of the continuous-energy Monte Carlo code Serpent [5] and based on previous investigations with cross sections generated by Serpent [6].

II. MYRRHA MINIMAL CRITICAL CORE

The MYRRHA minimum critical core generates a power of 80 MW_{th} and is composed of 52 fuel assemblies containing mixed oxide fuel (MOX), 6 control rods, 3 safety rods, 108 dummy LBE rods, and 42 beryllium reflector assemblies (see Fig. 1). Four different core configurations are analyzed in the present work:

- All Rods Out (ARO),
- All Rods In (ARI),
- Control Rods inserted in the core and Safety Rod extracted of the core (CR in/SR out),
- Control Rods extracted of the core and Safety Rod inserted in the core (CR out/SR in).

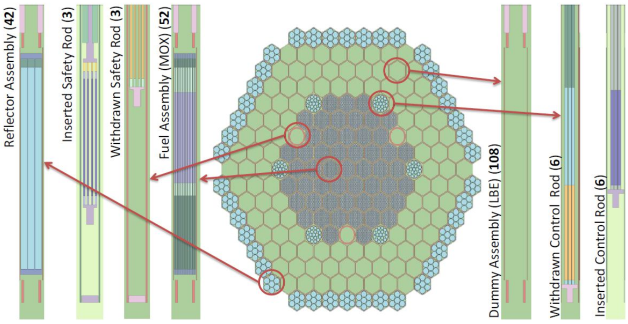

Fig. 1. Serpent whole core model: Vertical cross sections of different subassembly types and horizontal view of the core.

III. CODES AND MODELS

1. Multi-group cross section libraries for SCALE

The multi-group (MG) cross section libraries provided with SCALE 6.2 are optimized for systems with a thermal flux spectrum. The commonly used 252-group library, for example, was weighted with a light water reactor (LWR) pin cell neutron spectrum and shows a fine energy group structure in the resonance region. This library contains a limited number of energy groups in the fast energy range, but unnecessary energy groups in the thermal energy range for the analysis fast systems. In this context, new MG libraries have been generated and optimized for fast reactor systems. In a current study [7], a library with 302 energy groups and a weighting spectrum determined from a homogenized fuel assembly of a sodium-cooled oxide reactor core (302g MOX3600) was generated and lead to good results in fuel assembly criticality calculations. In addition to the application of this library, a MG library with 302 energy groups and the flux spectrum of the MYRRHA fuel assembly as weighting spectrum has been generated (302g MYRRHA). All of these libraries are based on ENDF/B-VII.1 data.

In order to assess the performance of the new MG libraries compared to the LWR library, and to investigate the influence of the applied weighting spectrum, criticality calculations of the fuel assembly are performed with the two-dimensional deterministic transport code NEWT and compared to corresponding reference calculations with the three-dimensional Monte Carlo code KENO; both codes are included in the SCALE 6.2 code package.

2. Macroscopic cross section generation with SCALE

Homogenized macroscopic cross sections in 8 energy groups [8] are generated using NEWT in combination with the previously mentioned multi-group libraries. Two-dimensional fuel assembly models with reflective boundary conditions are used for the generation of the macroscopic cross sections for the fuel assemblies which are located in the center of the core. For fuel assemblies located next to control rods or dummy assemblies, so-called super-cell models are applied: the fuel assembly is surrounded by the adjacent assemblies in order to take account a representative neutron flux with reflective boundary conditions. Four different fuel assemblies are identified: Fuel assemblies surrounded by:

- 1 control rod assembly and 5 fuel assemblies (see Fig. 2 left);
- 2 dummy assemblies and 4 fuel assemblies (see Fig. 2 right);
- 2 dummy assemblies, 1 control rod assembly and 3 fuel assemblies (see Fig. 3 left);
- 2 dummy assemblies, 1 control rod assembly, 1 safety rod assembly and 3 fuel assemblies (see Fig. 3 right).

The cross sections for the non-multiplying assemblies (e.g. control, safety, reflector assemblies etc.) are also generated by means of super-cell models: The assemblies are surrounded by fuel assemblies in an infinite lattice geometry (see Fig. 4).

Table I: Lower energy limits of the 8-group structure used with PARCS.

Group index	Lower limit [eV]	Group index	Lower limit [eV]
1	2.23E+06	5	4.09E+04
2	8.21E+05	6	1.50E+04
3	3.02E+05	7	7.49E+02
4	1.11E+05	8	1.00E-04

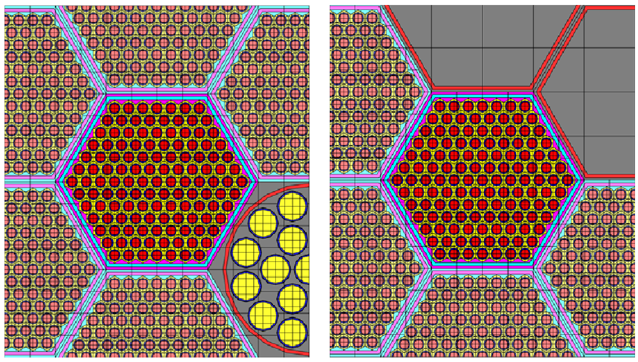

Fig. 2. NEWT super-cell models. Left: Fuel assemblies surrounded by 1 control rod assembly and 5 fuel assemblies; Right: Fuel assemblies surrounded by 2 dummy assemblies and 4 fuel assemblies.

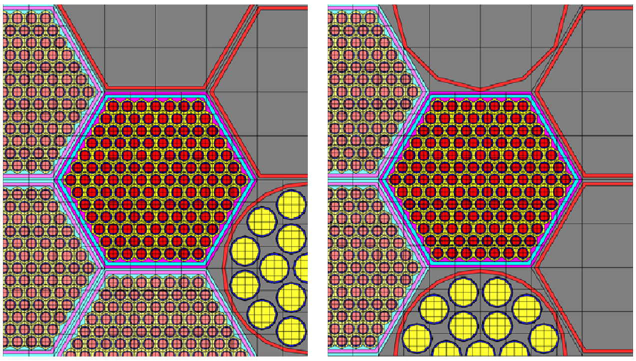

Fig. 3. NEWT super-cell models. Left: Fuel assemblies surrounded by 2 dummy assemblies, 1 control rod assembly and 3 fuel assemblies; Right: Fuel assemblies surrounded by 2 dummy assemblies, 1 control rod assembly, 1 safety rod assembly and 3 fuel assemblies.

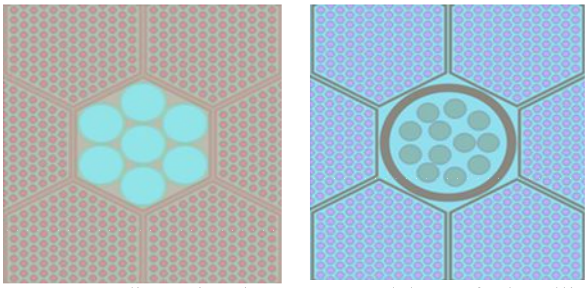

Fig. 4. Two-dimensional NEWT models. Left: beryllium reflector subassembly. Right: B4C safety rod subassembly.

3. Serpent model

Steady state models of the MYRRHA minimum critical core are developed for the continuous-energy Monte Carlo code Serpent 2.1.23. In order to be consistent with the multi-group cross section libraries used by the SCALE modules, the calculations are performed using the ENDF/B-VII.1 data library. The multiplication factors for the four configurations and the power distribution in the ARO configuration are assessed and used as references for the PARCS calculations.

With 200,000 neutrons in 2,000 active and 200 inactive cycles, the calculations with 20 MPI tasks last between 11 and 30 hours, depending on the configuration. The multiplication factors are converged to statistical errors of less than 5 pcm.

4. PARCS model

The generated macroscopic cross sections are used in whole-core calculations of the four configurations (ARO, ARI, CR in/SR out, CR out/SR in) with the nodal diffusion code PARCS. The subassemblies are divided into 1 radial node and between 54 and 57 axial nodes (depending on the configuration) in order to obtain fine results (the maximum mesh high is 5 cm). For all configurations, PARCS performs eigenvalue calculations.

IV. RESULTS

1. Multiplication factor of the fuel assembly

The multiplication factors for the reflected fuel assembly obtained with NEWT and KENO are compared in Table II. The NEWT calculations show a consistent underestimation of the KENO continuous-energy (CE) reference result by about 150 pcm. In contrast to similar studies with sodium-cooled fast reactor fuel assemblies [7], the new generated libraries do not result in improved results compared to the 252-group LWR library regarding the multiplication factor, and an influence of the weighting spectrum of the 302-group libraries is not visible.

The neutron flux spectra of these calculations are compared in Fig. 5 and Fig. 6. The neutron flux spectra obtained with NEWT and the 302-group libraries show large improvement towards the 252-group LWR library in comparisons with the corresponding reference KENO CE neutron flux (The displayed CE neutron flux was collapsed into the corresponding group structure for better comparison). The neutron flux spectra obtained with NEWT using the 302-group MOX3600 library and the 302-groups MYRRHA do not show significant differences; therefore only the flux with the 302g MYRRHA library is presented here. Since the neutron flux plays a major role for the generation of macroscopic few-group cross sections, the application of the new libraries for fast systems is considered as improvement towards the application of the LWR library.

Table II: Multiplication factors obtained with KENO and NEWT.

Code	KENO	NEWT	NEWT	NEWT
Library	CE	252g LWR	302g MOX3600	302g Myrrha
k_{inf}	1.57147	1.57517	1.57518	1.57553
$1/k_{MG}$-$1/k_{CE}$ [pcm]	(ref)	-150	-150	-164

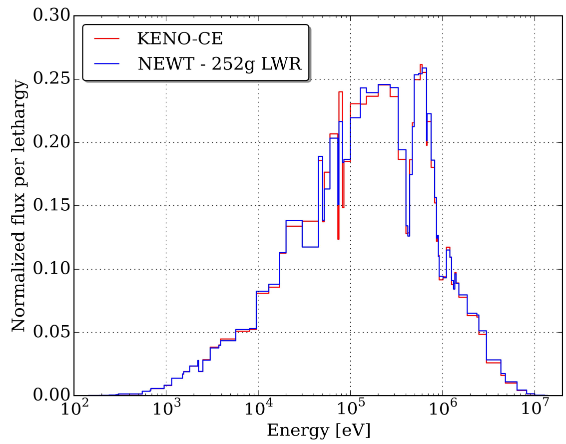

Fig. 5. Flux spectra in a MOX assembly in an infinite lattice compared between KENO CE and NEWT using the 252g LWR library.

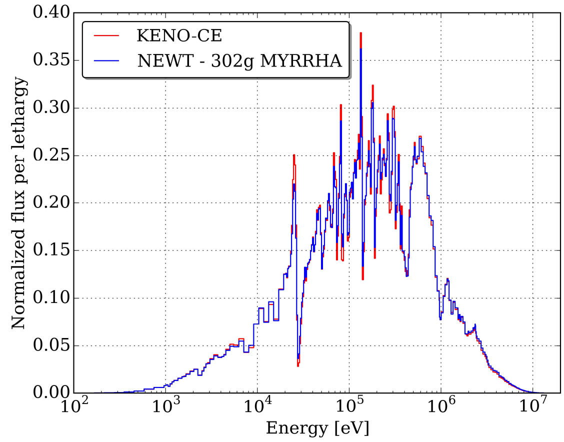

Fig. 6. Flux spectra in a MOX assembly in an infinite lattice compared between KENO CE and NEWT using the 302g MYRRHA library.

2. Multiplication factor of the full-core

Table III shows results obtained for the whole core simulations. It can be observed that the use of the 302g MOX3600 and 302g MYRRHA libraries does not lead to improved agreement with the Serpent reference result. In a previous study of the MYRRHA core [6], cross sections generated with Serpent and two-dimensional models have also lead to a similar disagreement regarding the multiplication factor. Those results were improved by applying three-dimensional models for the generation of the cross sections. Since NEWT is a two-dimensional code, this method of improvement is not possible. Instead, the so-called super-cell models are created to improve the cross section generation. Table IV shows results obtained for the whole core simulations without using the super-cell model, but with the single reflected fuel assembly model. The application of the super-cell models for the outermost fuel assemblies significantly improves the results for the ARO configuration, but the deviations for the other configurations remain greater than 800 pcm.

Table III: Comparison of multiplication factors between PARCS using various few-group cross sections prepared by SCALE compared to a reference Serpent calculation for four different core configurations.

		ARO	CR in/ SR out	CR out/ SR in	ARI
Serpent reference continuous-energy solution:					
Serpent	k_{eff}	1.01081	0.94810	0.97547	0.92440
PARCS using macroscop. cross sections prepared with SCALE:					
252g LWR	$\Delta\rho$ [pcm]	-269	-1071	-806	-1419
302g MOX3600	$\Delta\rho$ [pcm]	-276	-1199	-870	-1584
302g MYRRHA	$\Delta\rho$ [pcm]	-294	-1225	-892	-1611

Table IV: Comparison of multiplication factors between PARCS using various few-group cross sections prepared by SCALE without the super-cell model compared to a reference Serpent calculation for four different core configurations.

		ARO	CR in/ SR out	CR out/ SR in	ARI
Serpent reference continuous-energy solution:					
Serpent	k_{eff}	1.01081	0.94810	0.97547	0.92440
PARCS using macroscop. cross sections prepared with SCALE:					
252g LWR	$\Delta\rho$ [pcm]	-708	-1397	-1256	-1730
302g MOX3600	$\Delta\rho$ [pcm]	-796	-1579	-1402	-1947
302g MYRRHA	$\Delta\rho$ [pcm]	-822	-1607	-1430	-1976

3. Control and safety rods worth

Fig. 7 presents the control and safety rods worths calculated with Serpent and PARCS using different cross section sets for the three core configurations. The deviations of the PARCS results range from 500 pcm to 1100 pcm. There is no significant impact of the applied multi-group cross section library with NEWT on the control rod worth. In a previous study of the MYRRHA core [6], cross sections generated with Serpent using three-dimensional models lead to a discrepancy ranging from 300 pcm to 500 pcm. The three-dimension models do consequently also not significantly improve the results. A special treatment for the calculation of control rod cross section should be sought in the future.

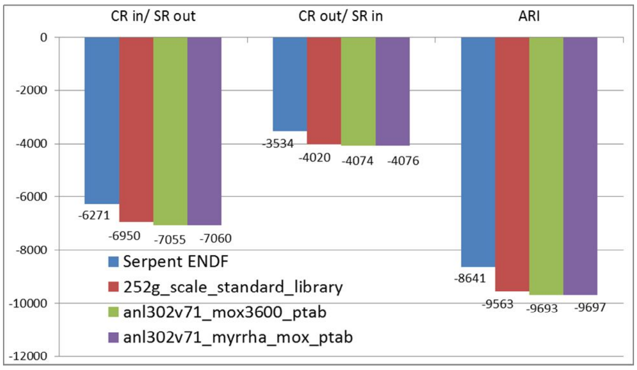

Fig. 7. Control and safety rod worths calculated by Serpent and PARCS using various few-group cross sections prepared by SCALE.

4. Radial power distribution

In this section, the power distribution calculated with PARCS using the three different cross section sets for the four core configurations is analyzed and compared to the Serpent core solution. It is observed that the use of the 302g MOX3600 and 302g MYRRHA libraries instead of the 252-group LWR library does not improve the agreement with the Serpent reference result.

A. ARO

Fig. 8, Fig. 9, and Fig. 10 show comparisons of the axially integrated assembly wise radial power distribution between the PARCS simulations using the cross section sets generated with the 252g, 302g MOX3600 and 302g MYRRHA libraries, respectively, with the Serpent reference calculation at the ARO core configuration. The three PARCS simulations result in almost consistent differences to the reference; the relative difference is thereby always below 4.3% which is acceptable (see Table V). This is the order of magnitude observed for LWR studies.

Table V: Maximum, minimum, Root Mean Square for the assembly wise radial power distribution comparison in ARO configuration.

	MAX	MIN	RMS
252g LWR	3.57	-1.70	1.76
302g MOX3600	4.26	-1.75	2.08
302g MYRRHA	4.30	-1.76	2.09

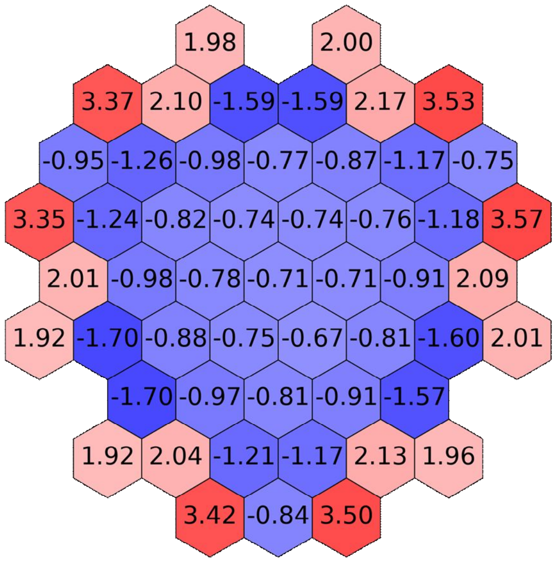

Fig. 8. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (252g LWR) of the ARO configuration.

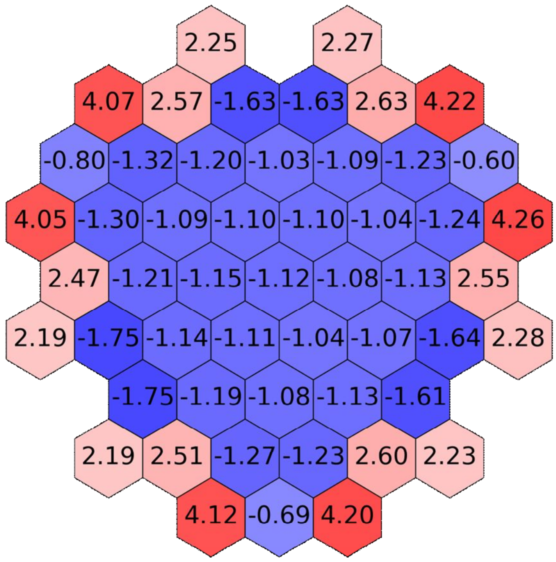

Fig. 9. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MOX3600) for the ARO configuration.

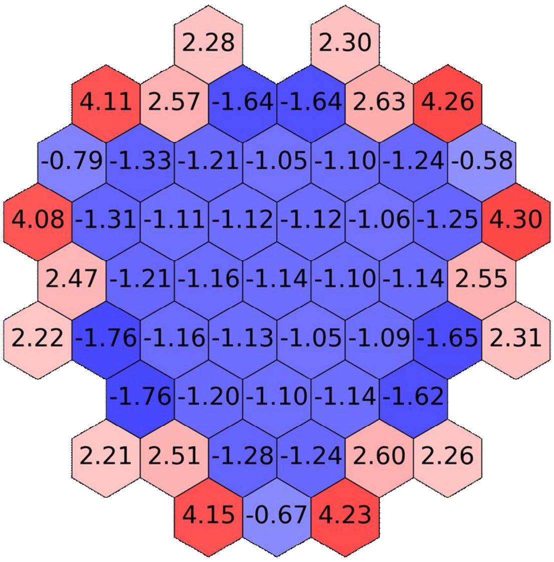

Fig. 10. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MYRRHA) for the ARO configuration.

B. CR in/SR out

Fig. 11, Fig. 12, and Fig. 13 show comparisons of the axially integrated assembly wise radial power distribution between the PARCS simulations using the cross section sets generated with the 252g, 302g MOX3600 and 302g MYRRHA libraries, respectively, with the Serpent reference calculation at the Control Rod In and Safety Rod Out core configuration. The three PARCS simulations result in consistent differences to the reference; the relative difference is thereby always below 2% which is better than in the ARO core configuration (see Table VI).

Table VI: Maximum, minimum, Root Mean Square for the assembly wise radial power distribution comparison in CR in/SR out configuration.

	MAX	MIN	RMS
252g LWR	1.40	-1.29	0.83
302g MOX3600	2.03	-1.32	1.06
302g MYRRHA	2.07	-1.33	1.08

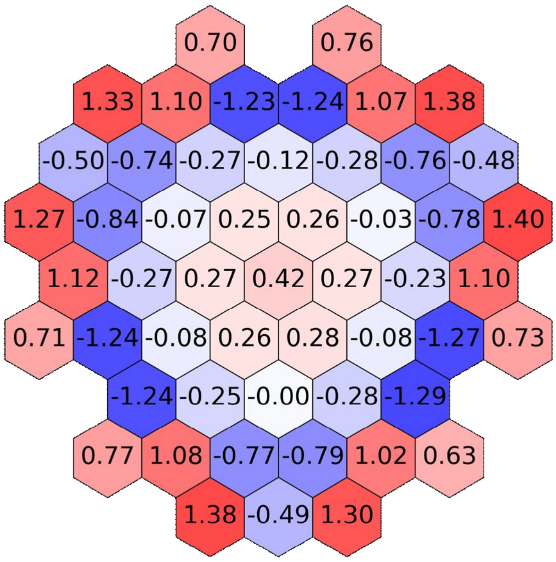

Fig. 11. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (252g LWR) of the CR in/SR out configuration.

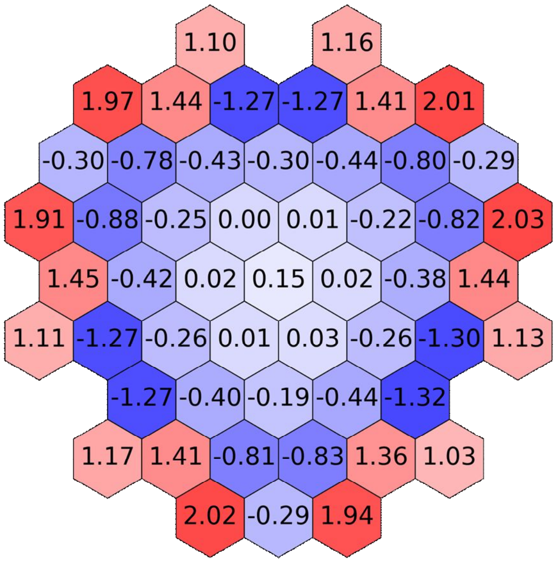

Fig. 12. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MOX3600) for the CR in/SR out configuration.

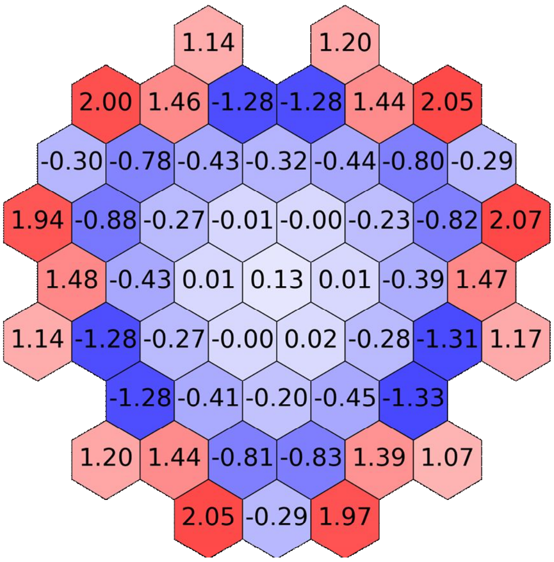

Fig. 13. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MYRRHA) for the CR in/SR out configuration.

C. CR out/SR in

Fig. 14, Fig. 15, and Fig. 16 show comparisons of the axially integrated assembly wise radial power distribution between the PARCS simulation using the cross section sets generated with the 252g, 302g MOX3600 and 302g MYRRHA libraries, respectively, with the Serpent reference calculation at the Control Rod Out and Safety Rod In core configuration. The three PARCS simulations result in consistent differences to the reference; the relative difference is thereby always below 4.3% which is comparable to the ARO core configuration (see Table VII).

Table VII: Maximum, minimum, Root Mean Square for the assembly wise radial power distribution comparison in CR out/SR in configuration.

	MAX	MIN	RMS
252g LWR	3.58	-2.22	1.58
302g MOX3600	4.28	-2.26	1.86
302g MYRRHA	4.31	-2.26	1.86

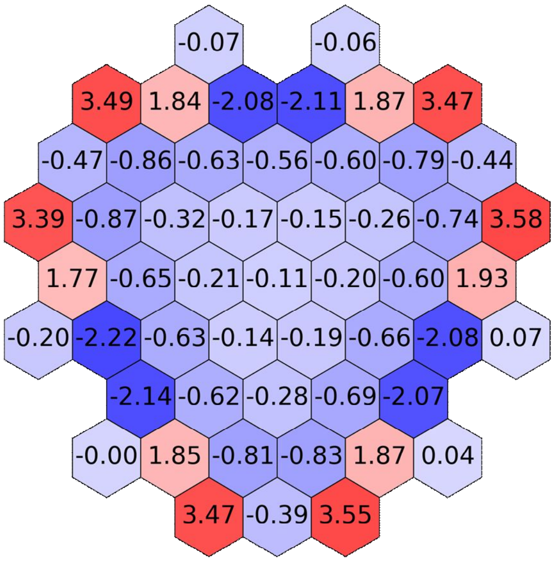

Fig. 14. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (252g LWR) of the CR out/SR in configuration.

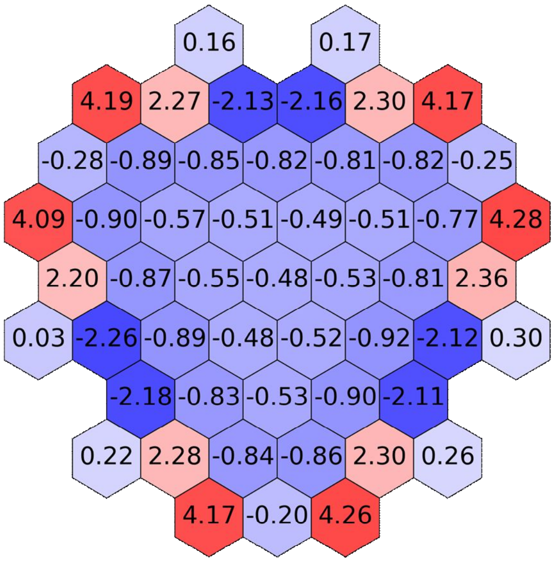

Fig. 15. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MOX3600) for the CR out/SR in configuration.

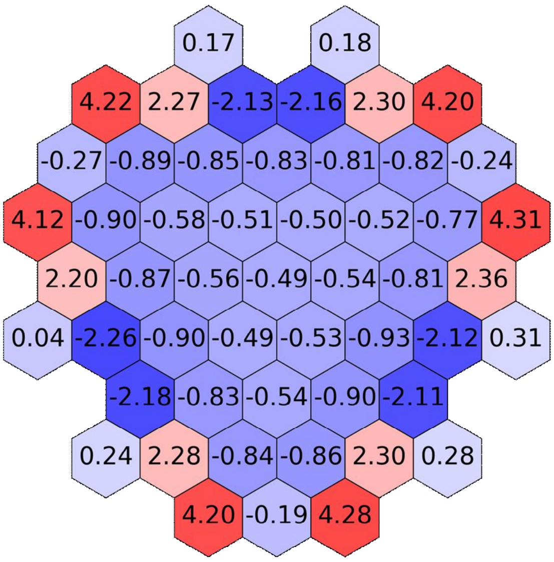

Fig. 16. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MYRRHA) for the CR out/SR in configuration.

D. ARI

Fig. 17, Fig. 18, and Fig. 19 show comparisons of the axially integrated assembly wise radial power distribution between the PARCS simulation using the cross section sets generated with the 252g, 302g MOX3600 and 302g MYRRHA libraries, respectively, with the Serpent reference calculation at the ARI core configuration. The three PARCS simulations result in almost consistent differences to the reference; the relative difference is thereby always below 2.3% which is better than the ARO core configuration (see Table VIII).

Table VIII: Maximum, minimum, Root Mean Square for the assembly wise radial power distribution comparison in ARI configuration.

	MAX	MIN	RMS
252g LWR	1.58	-1.70	0.97
302g MOX3600	2.22	-1.72	1.10
302g MYRRHA	2.27	-1.72	1.11

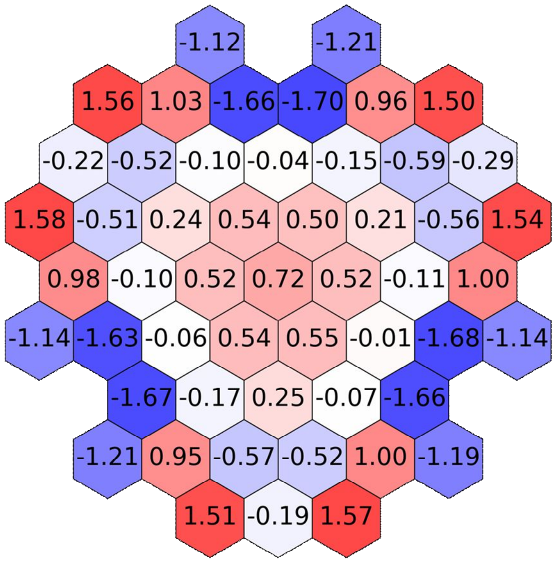

Fig. 17. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (252g LWR) of the ARI configuration.

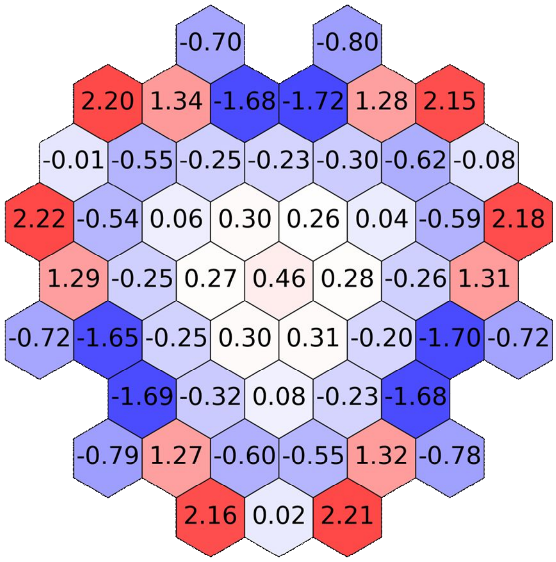

Fig. 18. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MOX3600) for the ARI configuration.

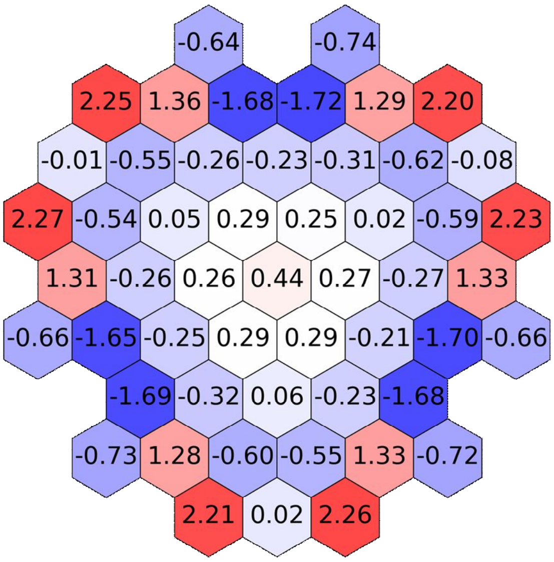

Fig. 19. Relative difference [%] of the axially integrated assembly wise radial power distribution between Serpent and PARCS/SCALE (302g MYRRHA) for the ARI configuration.

V. CONCLUSIONS

The NEWT code of the SCALE 6.2 code package is applied for the generation of macroscopic cross sections for use in whole-core calculations of the MYRRHA minimal critical core with the nodal diffusion code PARCS.

The 252-group library from SCALE 6.2 is weighted with a light water reactor spectrum, shows a fine energy group structure in the resonance region and contains a limited number of energy groups in the fast energy range. A library with 302 energy groups and a weighting spectrum determined from a homogenized fuel assembly of a sodium-cooled oxide reactor core (302g MOX3600) was generated. Another MG library with 302 energy groups and the flux spectrum of the MYRRHA fuel assembly as weighting spectrum has additionally been generated (302g MYRRHA).

At fuel assembly level, an influence of the weighting spectrum of the 302-group libraries is not visible on the multiplication factor. But the neutron flux spectra obtained with NEWT and the 302-group libraries show large improvement towards the 252-group LWR library in comparisons with the corresponding reference KENO CE neutron flux. Since the neutron flux plays a major role for the generation of macroscopic few-group cross sections, the application of the new libraries for fast systems is considered as improvement towards the application of the LWR library.

The macroscopic cross sections were generated with the three different libraries and used in the diffusion code PARCS to calculate the MYRRHA core at four different configurations. Comparisons in terms of the multiplication factor, control rod worth and the fuel assembly power are performed with Serpent Monte Carlo calculations. It is observed that the use of the 302g MOX3600 and 302g MYRRHA libraries does not improve the results in comparisons with the Serpent reference results.

Similar to previous studies with macroscopic cross sections generated by means of Serpent with two-dimensional models [6], large differences to the reference Monte Carlo whole-core calculation are observed. Since large improvements are obtained when using three-dimensional models in Serpent, the so-called super-cell models for cross section generation were applied in NEWT for the outermost fuel assemblies. In this model, the fuel assembly models are extended by adjacent assemblies to take into account a representative neutron flux. The generation of macroscopic cross sections using these super-cells leads to improved agreements on multiplication factor to the reference calculation for the ARO core configuration. However, this improvement could not be observed for controlled core configurations. Therefore, the deviation of the determined control rod worths to the reference solutions remains significant. This large deviation was, however, expected since earlier studies of the MYRRHA core using Serpent for macroscopic cross section generation using three-dimensional also resulted in large discrepancies. A special treatment for the calculation of control rod cross section should be sought in the future like for instance the use of SPH method performed in [10]. Nonetheless, the radial power distribution in the four core configurations calculated with PARCS are in good agreement with the reference Serpent solutions.

NOMENCLATURE

ARO = All Rod Out
ARI = All Rod In
CR in/SR out = Control Rod in/Safety Rod out
CR out/SR in = Control Rod out/Safety Rod in

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