M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

SCALE Multi-Group Libraries for Sodium-cooled Fast Reactor Systems

Friederike Bostelmann[1,3], Nicholas R. Brown[2], Andreas Pautz[3], Bradley T. Rearden[4], Kiril Velkov[1], Winfried Zwermann[1]

[1]*Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Boltzmannstraße 14, 85748 Garching, Germany*
[2]*Pennsylvania State University, Old Main, State College, PA 16801, USA*
[3]*École polytechnique fédérale de Lausanne, 1015 Lausanne, Switzerland*
[4]*Oak Ridge National Laboratory, P.O. Box 2008, Bldg. 5700, Oak Ridge, TN 37831-6170, USA*

friederike.bostelmann@grs.de, nrb26@psu.edu, andreas.pautz@epfl.ch, reardenb@ornl.gov, kiril.velkov@grs.de, winfried.zwermann@grs.de

Abstract - *As basis for systematic sensitivity and uncertainty analyses of fast spectrum systems with modules of the SCALE code package, new multi-group cross section libraries are generated considering typical hard neutron flux spectra and a sufficient resolution of the resonances in the fast energy. The performance of the new libraries is investigated in terms of the eigenvalue, the neutron flux and reaction rates in criticality calculations, and for the generation of group constants. The fuel assembly models utilized for these studies are borrowed from the specifications of two sodium-cooled fast reactors containing metal and oxide fuel, respectively, that are defined within the SFR-FT benchmark. To estimate the influence of geometrical effects within the self-shielding calculations, heterogeneous fuel assemblies are investigated as well as their homogenized variants and corresponding pin cells. Significant improvement compared to calculations with the available 252-group SCALE library are obtained in criticality calculations with a library including 302 energy groups and the flux spectrum of the homogenized oxide fuel assembly as weighting function. Slightly larger deviations to reference continuous-energy calculations are found in calculations of the heterogeneous oxide fuel assembly. Possible reasons are geometrical effects in the self-shielding calculations including the negligence of the fuel assembly wrapper. The applicability of the 302-group library is furthermore confirmed for the generation of macroscopic few-group cross sections; the comparison of generated 8-group constants with reference Serpent continuous-energy calculations leads to good agreement.*

I. INTRODUCTION

The Generation IV International Forum has identified sodium-cooled fast reactors as one of six most promising systems for the future[1]. Sodium-cooled fast reactor (SFR) technologies have been identified as potentially promising in both demonstration reactor and test reactor missions in the recent U.S. Department of Energy Office of Nuclear Energy (DOE-NE) Advanced Demonstration and Test Reactor (ADTR) Study[2]. Specifically, the ADTR study identifies SFRs as the most promising reactor technology option for demonstrating actinide management to extend natural resource utilization and reduce the burden of nuclear waste for future generations. Although only a few test and demonstration SFR facilities have been operated, this reactor concept is expected to play an increasing role for the generation of electricity in the future.

There is a growing interest and need to validate or adjust existing tools for adequate simulations of the reactor physics with fast neutron spectra. Several simulation sequences for reactor physics calculations are included in the SCALE code package[3]. In calculations with the one- and two-dimensional deterministic neutron transport codes XSDRN and NEWT, respectively, and the Monte Carlo code KENO, system parameters such as the multiplication factor and reactivity effects can be determined. NEWT moreover offers the possibility to generate homogenized few-group macroscopic cross sections for use in nodal diffusion codes. Additionally, potential sources of bias in the underlying nuclear data can be identified using SCALE tools. The energy dependence of these uncertainties can be better understood with tools for uncertainty and sensitivity analyses that use available neutron cross section covariance data.

The mentioned SCALE neutron transport codes apply multi-group (MG) cross sections; only KENO can also be used with continuous-energy (CE) cross sections. The multi-group libraries provided with SCALE for reactor physics analyses have been optimized for thermal systems. For example, they show a fine energy group structure in the resolved resonance region, but only a coarse structure in the fast region. In case of fast spectrum systems, there are, however, resonances caused by, for example, structural materials that need to be appropriately captured. Therefore, in order to perform scoping analyses of fast systems with SCALE, the generation of a new multi-group library optimized for fast spectrum systems is required.

In this study, a set of new multi-group libraries is generated in order to find a library that leads to sufficiently good agreement of multi-group calculations

with reference continuous-energy solutions. The libraries are tested in criticality calculations of fuel assemblies taken from sodium-cooled reactor cores that contain metal and oxide fuel, respectively. The intended end-use of these libraries is for cross section sensitivity and uncertainty analysis of fast reactor benchmark problems.

II. CALCULATION TOOLS AND MODELS

The models under investigation are taken from the OECD/NEA Sodium Fast Reactor Core Feedback and Transient Response (SFR-FT) Task Force definitions[4]. The specifications of one fuel assembly from the middle section of the inner core of the proposed medium-sized metallic fuel core (MET1000, cf. Fig. 1) and the large oxide core (MOX3600), respectively, are chosen for this study. The MOX3600 fuel pins contain annular U-TRU oxide pellets, and the MET1000 pins contain cylindrical U-TRU-Zr metal pellets. The fuel in both assemblies is beginning-of-equilibrium-cycle fuel. The cladding and the hexagonal wrapper tube for the MET1000 assembly are made of HT-9 steel, while the MOX3600 assembly includes EM-10 like steel and oxide strengthened steel (ODS), respectively. For the complete specifications it is referred to Ref. [4].

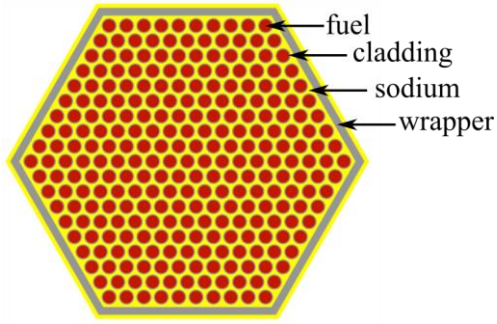

Fig. 1. MET1000 fuel assembly.

In preparation for the generation of new multi-group libraries, the neutron transport code CENTRM of SCALE is applied on volume-homogenized mixtures of the described fuel assemblies in order to obtain neutron flux distributions for use as weighting spectra for the multi-group cross sections. CENTRM computes pointwise neutron spectra for the homogenous infinite media up to an energy of 100 keV (user-specified input) by solving the Boltzmann transport equation using a combination of continuous-energy and multi-group nuclear data. Usually, these neutron spectra are used to generate self-shielded multi-group cross sections as input for neutron transport solvers. At higher energies, the neutron flux is obtained with the SCALE code BONAMI that performs Bondarenko calculations for resonance self-shielding.

In criticality calculations with the two-dimensional deterministic transport solver NEWT, simple square models containing these homogenized mixtures are furthermore used to study the influence of the new multi-group libraries on the multiplication factor, the multi-group neutron flux spectrum and reaction rate distributions while excluding any geometrical influence on the results. Problem-specific cross sections for NEWT are thereby obtained with CENTRM and BONAMI as described above. The MET1000 model is investigated at 293 K and at 900 K; the MOX3600 model is investigated at 293 K and 1500 K. The respective higher temperatures are chosen to be close to the specified fuel temperatures in the benchmark, but also to match temperatures for which cross sections are directly available in both the continuous-energy and multi-group libraries. In this way, any possible effect caused by additional temperature interpolation is excluded. As reference for comparison, calculations with the KENO-VI Monte Carlo Code with CE cross sections are performed.

The calculations of the homogenized models are followed by criticality calculations of the corresponding heterogeneous fuel pin cells and fuel assemblies for which temperatures according to the specifications are applied (cf. Table I). Problem-dependent cross sections are again obtained by CENTRM and BONAMI; the CENTRM pointwise flux is in both cases determined by a one-dimensional discrete ordinate solution of a fuel pin cell.

Table I: Temperatures applied in the heterogeneous models.

	MET1000	MOX3600
Fuel	807 K	1500 K
Cladding	706 K	743 K
Coolant	706 K	743 K
Wrapper	706 K	743 K

The new cross section library shall later be used for the generation of homogenized macroscopic few-group cross sections with NEWT for full core calculations with nodal diffusion codes. Therefore, the applicability of the 302-group library is tested for the generation of macroscopic 8-group[5] cross sections using the heterogeneous fuel assembly models. As reference for comparison, 8-group cross sections are additionally generated by the three-dimensional continuous-energy Monte Carlo code Serpent[6].

III. GENERATION OF MULTI-GROUP CROSS SECTION LIBRARIES

Several multi-group libraries with different energy group structures and weighting spectra are generated using the AMPX code system[7] provided with SCALE 6.2. All of them are based on ENDF/B-VII.1 data[8].

As it was already mentioned in the previous section, the neutron flux of the MET1000 and MOX3600 homogenized fuel assemblies generated with CENTRM

are chosen as weighting spectra for the new MG libraries. In Fig. 2, these spectra are compared with the base weighting function that is used for the 252-group SCALE library, the thermal neutron flux spectrum of a light water reactor (LWR) pin cell lattice. It can be clearly seen that due to the hard flux spectra of the SFR assemblies, a fine group structure as for the thermal region of the LWR library is not necessary for the studied systems. However, the new libraries need to contain more energy groups between about 10^4 and 10^6 eV to appropriately capture the resonances in this region.

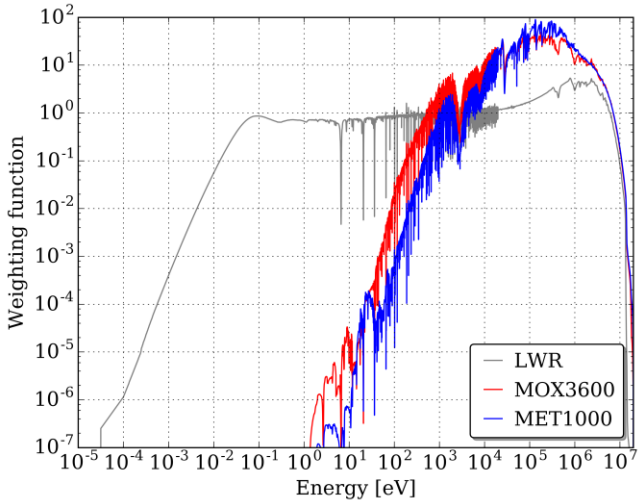

Fig. 2. Weighting spectra of the multi-group libraries.

Table II: Overview of the generated multi-group cross section libraries. Group structures indicated with an asterisk are directly taken from the MC^2-3 libraries.

Number of groups	Weighting spectrum
230*	MET1000, MOX3600
245	MOX3600
253	MOX3600
271	MOX3600
302	MET1000, MOX3600
425*	MET1000, MOX3600
2082*	MET1000, MOX3600

For first investigations, group structures optimized for fast spectrum systems used in the DOE-NE Advanced Reactor Technologies (ART) program and in particular the MC^2-3 code[9] are chosen. The MC^2-3 libraries of interest contain 230, 425, and 2082 energy groups. For the finest 2082 group structure, the energy range between 0.414 eV and 14.191 MeV is divided into 2082 equal lethargy bins. The other group structures are subsets of this fine structure. In order to find a library that leads to reasonable results with a minimal number of groups to keep the computation time at a minimum, combinations of these group structures are tested (cf. Table II). In particular, boundaries of the 425-group structure were added to the 230-group structure in order to include a finer resolution of occurring resonances. In Fig. 3, the MOX3600 weighting spectrum collapsed into the 2082-, 302- and 230-group structure is presented to visualize the finer energy group structure in the fast region compared to the LWR library. This plot furthermore shows the energy range in which additional group boundaries from the 425-group structure were added the 230-group structure to generate the 302-group structure.

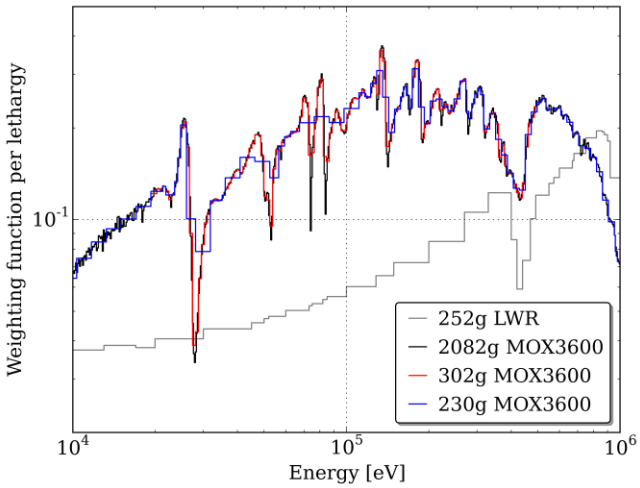

Fig. 3. Weighting spectra collapsed into multi-group structures; energy range in which group boundaries of the 425-group structure are added to the 230-group structure to obtain the 302-group library.

IV. RESULTS

This section presents the comparison of NEWT multi-group calculations with corresponding KENO-VI continuous-energy reference solutions in order to assess the performance of the new generated multi-group libraries for the fast reactor systems under investigation.

1. Criticality calculations of homogenized fuel assemblies

Table III presents the differences of the obtained multiplication factors with NEWT using various multi-group libraries compared to the reference KENO CE solution at 293 K. The results in this table as well as in the following figures are only displayed for 293 K since the results for the respective higher temperature are very similar. It can be clearly seen that the 252-group SCALE library shows a significant disagreement regarding the multiplication factor. This disagreement can also be observed when comparing the corresponding flux distribution in Fig. 4 and therefore emphasizes the need for an additional SCALE library optimized for fast neutron spectra.

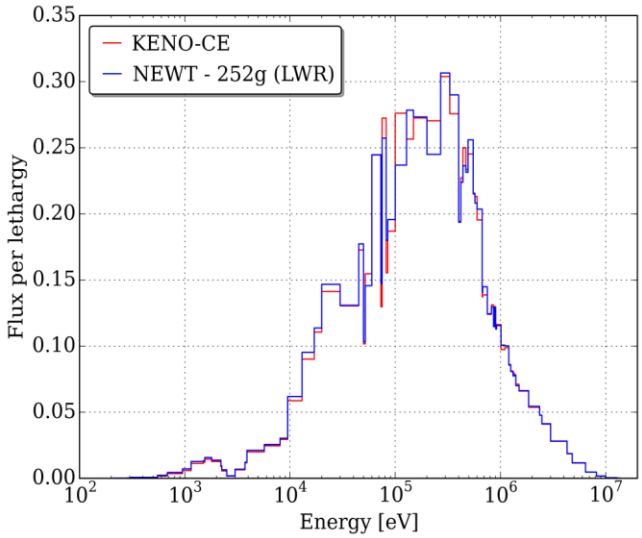

Fig. 4. Neutron flux distribution of the homogenized MET1000 fuel assembly at 293 K determined with the 252g LWR library compared to the reference CE solution (linear scale).

For 230, 302, 425 and 2082 energy groups, calculations with both the MET1000 and the MOX3600 weighting spectrum can be compared. For the oxide fuel, the influence of the weighting spectra is negligible with less than 10 pcm. Only slightly larger effects can be observed for the metallic fuel, with the maximum difference of 55 pcm for 230 groups. In a side study, the 230- and 425-group libraries are also generated with the Watt fission spectrum of Pu-239 as weighting function. This spectrum is a smooth function; it does not contain the typical jagged distribution in the fast energy range and is therefore considered as inadequate for the intended analyses. However, the maximum difference of the results with this library compared to corresponding calculations with the MET1000 and MOX3600 weighting spectra is still less than 100 pcm. This result supports the suggestion that the number of energy groups might already be large enough such that the influence of the weighting spectrum is small for the considered systems.

The finest considered libraries contain 2082 groups. Since this is a very fine structure and geometrical effects are excluded because of the homogenization, NEWT calculations with these libraries are expected to result in the best agreement with the corresponding continuous-energy reference solution. This is indeed the case for the oxide fuel where the deviation is reduced to 10 pcm. In contrast, the 230-group library leads to a deviation only slightly improved compared to the LWR library. When gradually adding groups to the 230-group library, the deviation to the reference decreases. It seems that already the 302-group structure is sufficient to provide reasonable agreement with the reference regarding the multiplication factor; the finer 425-group structure does not provide a significantly better result.

For the metallic fuel, the 2082-group calculations lead to a multi-group bias of about 70 pcm. Although the 245 and 253-group libraries lead to agreement regarding the multiplication factor, it is assumed that this is caused by error cancellation effects. The best result is therefore considered to be obtained with the 302-group structure and the MOX3600 weighting spectrum because this result shows good agreement with the expected multi-group bias.

Table III: Reactivity difference between NEWT MG and reference KENO CE solutions for the homogenized fuel assemblies at 293 K. The 1σ standard deviation of the KENO CE solution is less than 5 pcm.

MG library	$\Delta\rho = (1/k_{ref} - 1/k_{\infty})$ [pcm]	
	MET1000	MOX3600
252g, LWR	-253	167
230g, MET1000	95	134
230g, MOX3600	40	126
245g, MOX3600	3	76
253g, MOX3600	0	58
271g, MOX3600	-48	40
302g, MET1000	-29	16
302g, MOX3600	**-65**	**23**
425g, MET1000	-37	13
425g, MOX3600	-62	14
2082g, MET1000	-64	-9
2082g, MOX3600	-73	-10

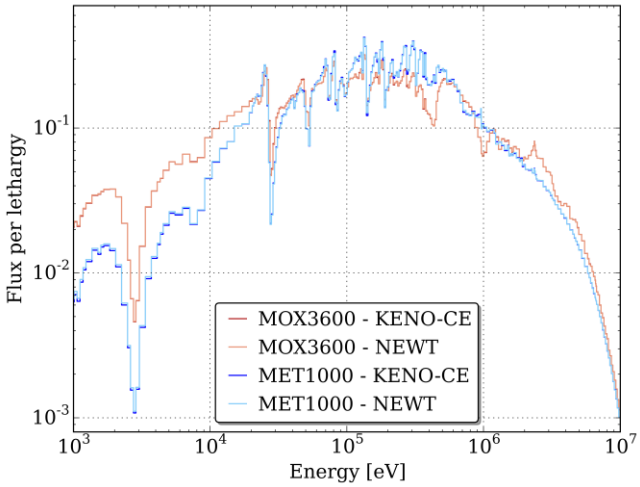

Fig. 5. Neutron flux distribution of the homogenized fuel assemblies at 293 K in the fast energy range; the NEWT calculations are performed with the 302-group library using the MOX3600 weighting spectrum (logarithmic scale).

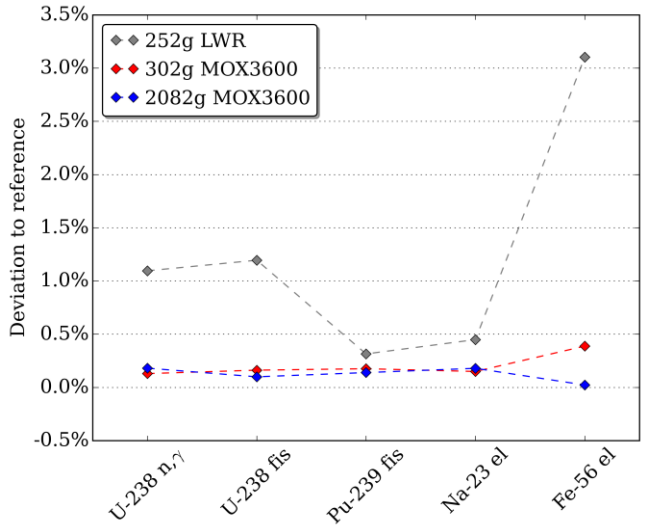

Fig. 6. Collapsed one-group cross sections of the homogenized MET1000 fuel assembly at 293 K compared to the CE reference.

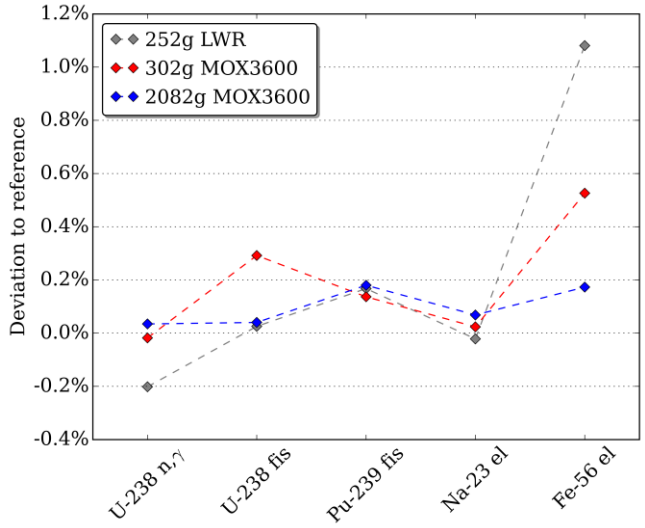

Fig. 7. Collapsed one-group cross sections of the homogenized MOX3600 fuel assembly at 293 K compared to the CE reference (Note the different scale compared to Fig. 6).

The good agreement with the 302-group MOX3600 library can also be observed for the flux spectra (cf. Fig. 5) and reaction rate distributions (cf. Fig. A.1 – Fig. A.4 in the appendix). For a meaningful comparison, the KENO CE results are collapsed to match the multi-group structure of the compared NEWT output. In order to compare not only distributions but also cumulative values, NEWT is applied to collapse the problem-dependent cross sections one-group cross sections. Fig. 6 and Fig. 7 compare a selection of these cross sections to the corresponding KENO CE reference values. The strong improvement compared to the 252-group LWR library is clearly visible. Especially for the capture cross section of U-238, which plays an important role for the temperature feedback, the difference of the 302-group MOX3600 calculation to the reference is decreased from about 1.01%/0.2% to less than 0.13%/0.02% for the MET1000/MOX3600 models, respectively.

2. Criticality calculations of heterogeneous fuel pin cells

The first investigated heterogeneous model is a fuel pin cell in an infinite triangular lattice for each of the considered assembly types. It is worthwhile mentioning again that, in contrast to the investigation of the homogenized model, the resonance self-shielding calculation with BONAMI and CENTRM is performed on a one-dimensional fuel pin cell, and the model for the transport calculation with NEWT is a two-dimensional model corresponding to the one-dimensional self-shielding model.

The multiplication factors between NEWT and KENO are compared in Table IV. The 2082-group calculations suggest a multi-group bias of about 100 and 40 pcm for the MET1000 and MOX3600 fuel pin, respectively. Apparently, the addition of a geometrical heterogeneity to the model leads to a slightly increased bias compared to the homogenized models. With about 30 pcm, this additional effect is, however, considered to be small. The calculations with the 302g MOX3600 library show reasonable agreement with the 2082-group calculations; this library is therefore considered as adequate for the simulation of these models. The corresponding flux and reaction rate distributions are not presented here because they show the same good agreement with the reference as for the homogenized model.

Table IV: Reactivity difference between NEWT MG and the reference KENO CE solution for the heterogeneous fuel pin cells. The 1σ standard deviation of the KENO CE solution is less than 5 pcm.

MG library	$\Delta\rho = (1/k_{ref} - 1/k_{\infty})$ [pcm]	
	MET1000	MOX3600
252g, LWR	-218	165
230g, MET1000	44	94
230g, MOX3600	-2	90
302g, MET1000	-75	-47
302g, MOX3600	**-92**	**-43**
425g, MET1000	-85	-21
425g, MOX3600	-104	-22
2082g, MET1000	-105	-37
2082g, MOX3600	-109	-38

3. Criticality calculations of heterogeneous fuel assemblies

The heterogeneous fuel assemblies of both core designs are investigated in two-dimensional criticality calculations with NEWT. The major difference to the fuel pin cell calculations is the additional wrapper (mostly iron and chromium) around the pins. Since the self-shielding calculation for the hexagonal lattices is currently limited to one dimension, it is not possible to consider this wrapper. The problem-dependent cross sections are therefore determined with the one-dimensional pin cell models as before. These cross sections are then applied with NEWT on the actual model including the wrapper. The comparison of the NEWT results with the reference KENO CE results is presented in Table V.

Table V: Reactivity difference between NEWT MG and the reference KENO CE solution for the heterogeneous fuel assemblies. The 1σ standard deviation of the KENO CE solution is less than 10 pcm.

MG library	$\Delta\rho = (1/k_{ref} - 1/k_{\infty})$ [pcm]	
	MET1000	MOX3600
252g, LWR	-43	437
230g, MET1000	296	394
230g, MOX3600	232	377
302g, MET1000	111	235
302g, MOX3600	**84**	**232**
425g, MET1000	95	225
425g, MOX3600	66	215
2082g, MET1000	*(not converged)*	*(not converged)*
2082g, MOX3600	7	104

For the metallic fuel assembly, the 2082-group NEWT calculation results in very good agreement with the reference. The calculation with 302 groups results in a deviation in the range of 100 pcm, which is considered as reasonable agreement. The 302-group library is therefore also considered here as appropriate for the metallic fuel assembly calculation. It shall be mentioned that the 252-group LWR library leads to smaller differences compared to the 302-group library regarding the multiplication factor. However, larger differences regarding the flux distribution with this library as already presented in Fig. 4 for the homogenized assembly can be observed.

For the oxide fuel assembly, larger deviations are observed. The increase of the number of groups from 302 to 2082 leads to an improvement of the multiplication factor of about 100 pcm. However, also the 2082-group calculation does not show an agreement with the reference as good as for the homogeneous mixture; it differs by about 100 pcm to the KENO calculation. This is in contrast to the results obtained with the homogenized fuel assembly. Since the fuel assembly only differs by the additional assembly duct to the fuel pin calculations, the increased deviation is probably caused by the negligence of the additional structural material in the self-shielding calculation.

For both systems, the influence of the weighting spectrum is negligible.

4. Generation of homogenized macroscopic few-group cross sections

The applicability of the 302-group library for the generation of homogenized macroscopic few-group cross sections is tested by comparing generated 8-group cross sections with corresponding Serpent results. The 8-group structure is taken from reference [5]; the individual boundaries are, however, slightly different to coincide with boundaries of the 252-group SCALE and 302-group library (cf. Table VI), respectively. The Serpent macroscopic cross sections are obtained accordingly, and they are converged such that their relative 1σ statistical error is about 0.01% or less in group 1-7 and up to 0.05% in group 8, the lowest energy group.

Table VI: The 8-group structure adjusted for boundaries of the 302-group library.

Group	Upper energy	Group	Upper energy
1	20 MeV	5	111.09 keV
2	2.2313 MeV	6	39.859 keV
3	820.85 keV	7	15.034 keV
4	301.97 keV	8	0.74852 keV

In contrast to the results of the criticality calculations, the comparisons of the 8-group cross sections seem not to be sensitive towards the multi-group library. The calculations with the 252-group SCALE library and the new 302-group library lead to similar differences to the reference Serpent results (cf. Fig. 8 – Fig. 11). With both libraries, differences of less than 1% are obtained in the fastest four energy groups and in the other groups the differences are less than 4%.

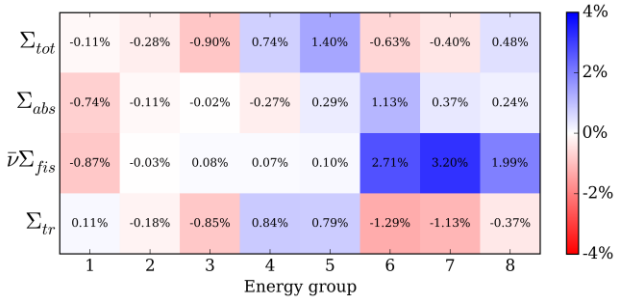

Fig. 8: Macroscopic 8-group cross sections generated with NEWT using the 252g library compared to Serpent for the MET1000 fuel assembly.

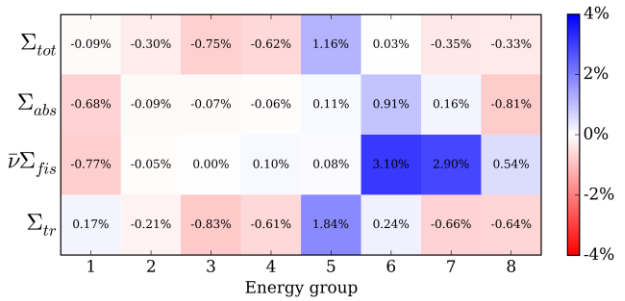

Fig. 9: Macroscopic 8-group cross sections generated with NEWT using the 302g library compared to Serpent for the MET1000 fuel assembly.

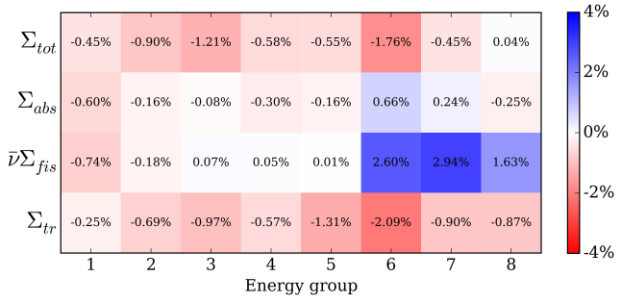

Fig. 10: Macroscopic 8-group cross sections generated with NEWT using the 252g library compared to Serpent for the MOX3600 fuel assembly.

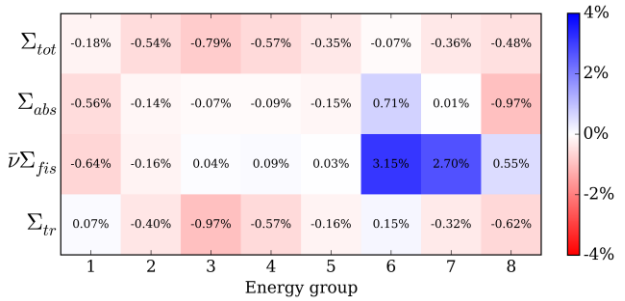

Fig. 11: Macroscopic 8-group cross sections generated with NEWT using the 302g library compared to Serpent for the MOX3600 fuel assembly.

5. Comparison of criticality calculations with Serpent

For the sake of completeness, the eigenvalues are also compared between KENO-VI and Serpent continuous-energy calculations (cf. Table VII). The eigenvalues for both the homogenized and the heterogeneous fuel assembly show differences of a few hundred pcm. This difference is first of all caused by differences in the applied probability tables for resonances in the unresolved energy range. Although the tables are in both cases based on identical ENDF data files, there are differences due to the processing. This is currently under investigation by the SCALE-Team[10]: If the probability tables are not applied or if the SCALE tables are modified to be consistent with the tables used by Serpent, both codes show reasonable agreement. The impact of the different probability tables on the neutron flux distribution is in contrast very small; the neutron flux distributions show very good agreement (cf. Fig. 12). This is also valid for the comparison with corresponding flux spectra determined with NEWT, whereas for these calculations the deviation to the Serpent eigenvalues is even larger.

Table VII: Reactivity difference between Serpent and KENO-VI both using CE cross sections. The statistical error is given in parentheses.

Model	$\Delta\rho = (1/k_{KENO} - 1/k_{Serpent})$ [pcm]	
	MET1000	MOX3600
homog. fuel assembly	-270(9)	-467(5)
heterog. fuel assembly	-244(4)	-451(7)

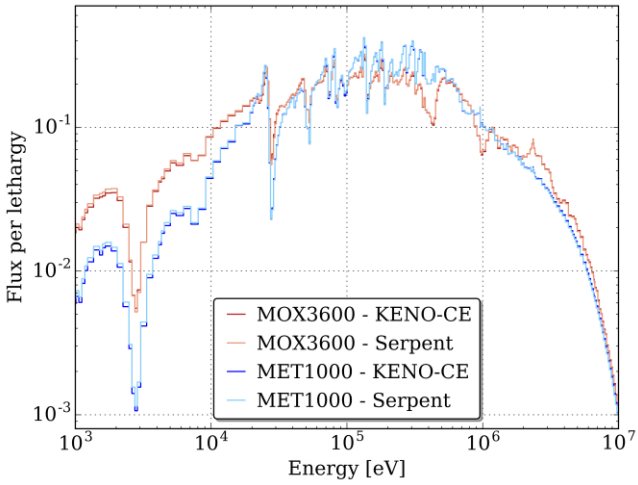

Fig. 12: Total neutron flux distribution of the heterogeneous fuel assemblies in the fast energy range; for better comparison, the results are collapsed into the 302-group structure.

6. Computation time

The intended end-use of the generated library is for uncertainty and sensitivity analysis. In case of random sampling based analyses, the transport calculation is repeated a large number of times with perturbed input parameters. Hence, during the generation of a new library for this purpose, the computation time for an individual calculation plays a significant role. In Table VIII, the computation times for various exemplary calculations are displayed. The computation times of the homogenized fuel assemblies are omitted here because most of them are in the range of less than half a minute and are therefore significantly biased by the current traffic on the computing cluster. For the same reason, the displayed times can only be considered as rough estimates.

The computation time of course scales with the number of energy groups in the library. It can be observed that the 252-, 230-, and 302-group calculations take about the same time. The 425-group calculations are a bit longer, and the 2082-group calculations are significantly longer such that random sampling based uncertainty analyses with these libraries are not considered practical.

After considering the computation time and sufficiently good agreement of the results for the metallic and the oxide fuel assemblies, it is concluded that the 302-group library with the oxide weighting function is chosen as the library with which the studies shall be continued.

Table VIII: NEWT computation time (in seconds).

MG library	Heterogeneous fuel pin		Heterogeneous fuel assembly	
	MET 1000	MOX 3600	MET 1000	MOX 3600
252g, LWR	128 s	236 s	184 s	543 s
230g, MOX3600	97 s	219 s	162 s	497 s
302g, MOX3600	98 s	217 s	208 s	544 s
425g, MOX3600	152 s	259 s	276 s	658 s
2082g, MOX3600	925 s	996 s	8820 s	9541 s

V. CONCLUSIONS

For reactor physics analyses of fast spectrum systems, modules of the SCALE code package in combination with multi-group cross sections shall be used. For this purpose, new multi-group cross section libraries were generated under consideration of the hard neutron flux spectra and a sufficient resolution of the resonances in the fast energy range of the systems of interest.

For criticality calculations of homogenized and heterogeneous fuel assemblies and the corresponding pin cells of a sodium-cooled fast reactor including metal and oxide fuel, respectively, a significant improvement compared to calculations with the 252-group SCALE library was found with a library including 302 energy groups and the pointwise spectrum of the homogenized oxide fuel assembly as weighting function. Reasonable agreement with reference solutions was found for the multiplication factor, the neutron flux and reaction rates. In most cases, the weighting function has only a small influence on the results due to a large number of energy groups.

Slightly larger deviations to the reference were found for calculations of the heterogeneous MOX3600 fuel assembly. Possible reasons are geometrical effects in the self-shielding calculations including the negligence of the fuel assembly wrapper. In subsequent studies, it will be investigated if better improvement can be obtained if the problem-dependent cross sections for the fuel pins adjacent to the wrapper are determined in a self-shielding calculation that includes an artificial outer wrapper layer around the one-dimensional fuel pin to consider additional effects such as the neutron scattering on structural material.

The applicability of the 302-group library in calculations for the generation of macroscopic few-group cross sections for use in nodal diffusion codes was confirmed in comparisons with reference Serpent continuous-energy calculations. The application of the new library did not lead to a significant improvement compared to calculations with the 252-group SCALE library; both libraries result in good agreement with the reference. In subsequent studies, it will be investigated whether there is an improvement due to the application of the new library in full core nodal diffusion calculations. Full core calculations of lead-bismuth cooled MYRRHA configurations based on few-group cross sections generated with NEWT and the 302-group library already indicate that the influence of the multi-group library might be negligible (presented at this conference)[11].

The study presented in this paper provides the basis for systematic sensitivity and uncertainty analyses of fast reactor systems. Pin cell and fuel assembly calculations will be followed by the analysis of uncertainties in full core calculations. Where possible, the perturbation theory-based TSUNAMI code of SCALE shall be applied. Furthermore, for all steps, the XSUSA code (Cross Section Uncertainty and Sensitivity Analysis)[12,13] with the random sampling approach will be applied to perturb the cross sections that serve as input for SCALE transport codes. Although the influence of the new multi-group library for macroscopic cross section generation and therefore for full core calculations might be small, it is expected that this library leads to significant improvement in pin cell and fuel assembly uncertainty and sensitivity analyses. The investigation of the performance of this new library compared to continuous-energy solution will therefore be extended to corresponding uncertainty and sensitivity calculations. The performance of the new multi-group library will furthermore be tested in calculations of experiments from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP Handbook)[14].

ACKNOWLEDGMENTS

This work is supported by the German Federal Ministry for Economic Affairs and Energy. The assistance of the SCALE-Team, especially Doro Wiarda and Mark L. Williams, during the generation of the multi-group libraries is greatly appreciated.

APPENDIX A: REACTION RATE DISTRIBUTIONS

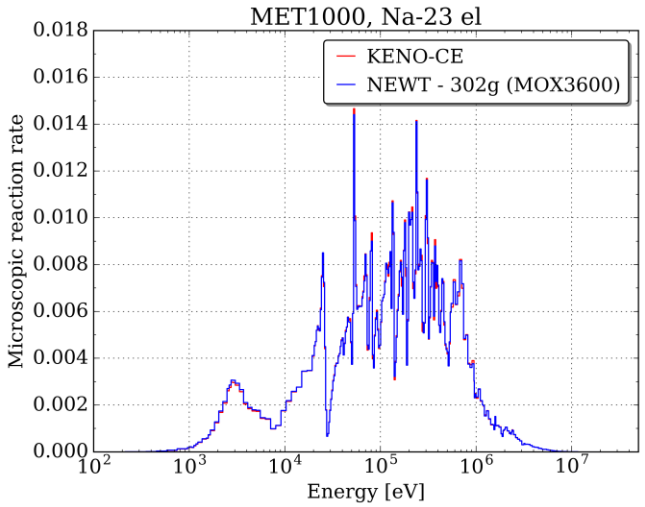

Fig. A.1. Elastic scattering of Na-23 in the homogenized MET1000 fuel assembly at 293 K.

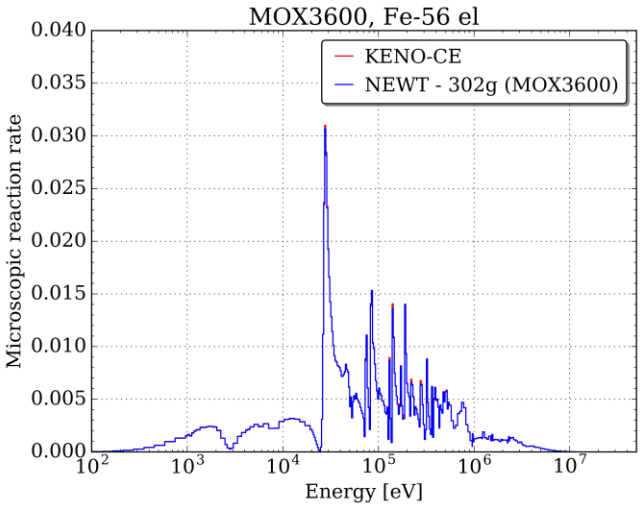

Fig. A.2. Elastic scattering of Fe-56 in the homogenized MOX3600 fuel assembly at 293 K.

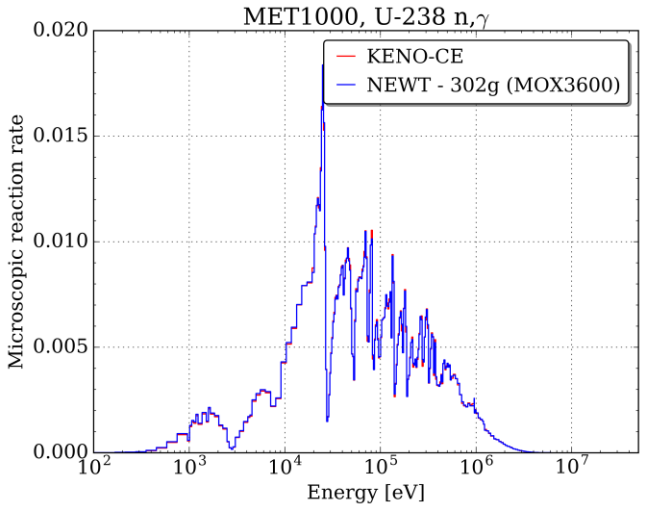

Fig. A.3. Neutron capture of U-238 in the homogenized MET1000 fuel assembly at 293 K.

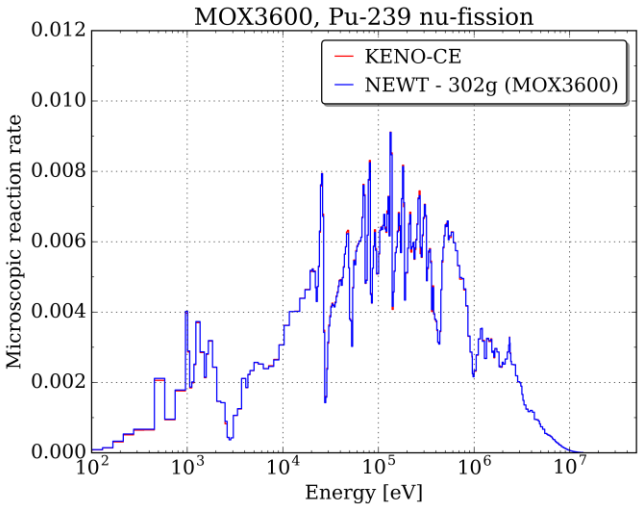

Fig. A.4. Neutron production of Pu-239 in the homogenized MOX3600 fuel assembly at 293 K.

REFERENCES

1. J. E. KELLY, "Generation IV International Forum: A decade of progress through international cooperation," *Progr. Nucl. Energy*, **77**, pp. 240–246, 2014.
2. D. PETTI, R. HILL, J. GEHIN, H. GOUGAR, G. STRYDOM, F. HEIDET, J. KINSEY, C. GRANDY, A. QUALLS, N. BROWN, J. POWERS, E. HOFFMAN, D. CROSON, "Advanced Demonstration and Test Reactor Options Study," INL/EXT-16-37867, Rev. 2, July 2016.
3. B.T. REARDEN and M.A. JESSEE, Eds., "SCALE Code System," ORNL/TM-2005/39, Version 6.2, Oak Ridge National Laboratory, Oak Ridge, TN (2016). Available from Radiation Safety Information Computational Center as CCC-834.
4. OECD/NEA, "Benchmark for Neutronic Analysis of Sodium-cooled Fast Reactor Cores with Various Fuel Types and Core Sizes," NEA/NSC/R(2015)9, February 2016.
5. A. E. WALTAR, D. R. TODD, P. V. TSVETKOV, "Appendix F: 4-Group and 8-Group Cross sections" *in* "Fast Spectrum Reactors", p. 643, Springer, 2012.

6. J. LEPPÄNEN, et al., "The Serpent Monte Carlo code: Status, development and applications in 2013", Annals of Nuclear Energy, Vol. 82, pp. 142-150, 2015.
7. D. WIARDA, M. E. DUNN, N. M. GREENE, C. CELIK, and L. M. PETRIE, "AMPX-6: A Modular Code System for Processing ENDF/B," ORNL/TM-2016/43, Oak Ridge National Laboratory, Oak Ridge, TN (2016). Available from Radiation Safety Information Computational Center as CCC-834.
8. M. B. CHADWICK, et al., "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data," *Nuclear Data Sheets*, **112**, pp. 2887–2996, 2011.
9. C. H. LEE, W. S. YANG, "MC²-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis," ANL/NE-11-41, Ref.1, January 31, 2012.
10. A. HOLCOMB, *private communication*, Feb. 2017.
11. J. BOUSQUET, F. BOSTELMANN, K. VELKOV, W. ZWERMANN, "Macroscopic Cross Section Generation with SCALE 6.2 for the MYRRHA Minimal Critical Core", *Proc. M&C2017*, Jeju, Korea, April 16–20, 2017.
12. F. BOSTELMANN, W. ZWERMANN, B. KRZYKACZ-HAUSMANN, L. GALLNER, A. AURES, K. VELKOV, "Sampling-Based Nuclear Data Uncertainty Analysis in Criticality and Depletion Calculations," in *Proc. ANS MC2015*, Nashville, Tennessee, USA, April 19–23, 2015.
13. M.L. WILLIAMS, G. ILAS, M.A. JESSEE, B.T. REARDEN, D. WIARDA, W. ZWERMANN, L. GALLNER, M. KLEIN, B. KRZYKACZ-HAUSMANN, A. PAUTZ, "A Statistical Sampling Method for Uncertainty Analysis with SCALE and XSUSA," *Nucl. Techn*. **183**, pp. 515–526, 2013.
14. NEA, "International Criticality Safety Benchmark Experiment Handbook," NEA-1486/14, September 2015.