Representation of the few-group homogenized cross sections of a MOX fuel assembly

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Abstract. Nodal diffusion methods are often used to calculate the distribution of neutrons in a nuclear reactor core. They require few-group homogenized neutron cross sections for every heterogeneous sub-region of the core. The homogenized cross sections are pre-calculated at various reactor states and represented in a way that facilitates the reconstruction of cross sections at other possible states. In this study a number of such representations were built for the cross sections of a MOX (mixed oxide) fuel assembly via hierarchical Lagrange interpolation on Clenshaw-Curtis sparse grids. Traditionally, nodal reactor core simulators have employed cross sections with two energy groups, but there is evidence that more energy groups are needed to simulate reactor cores that contain MOX. Representations were therefore constructed for both the traditional two energy groups and a six energy group structure. Both the rate at which the representation accuracy improves with the number of samples and the complexity of the cross section dependence on individual state parameters were examined. The anisotropy feature of the representation procedure, which allows more samples to be taken for state parameters that are known to be more important to the representation accuracy than others, was applied throughout. The results show that the representation method allows both two-group and six-group cross sections to be represented in a computationally efficient manner to an industrially acceptable level of accuracy, despite additional complexity in the dependence of six-group cross sections on the state parameters.

1. Introduction

Plutonium is produced in reactors that use low-enriched uranium oxide (UOX) fuel through the transmutation of uranium. The fissile isotope $^{239}_{94}$Pu can be recovered from spent UOX fuel and included during the fabrication of new fuel assemblies, which are then known as mixed oxide (MOX) fuel. Many pressurized water reactors (PWRs) load at least a part of the reactor core with MOX fuel, but this affects the neutron distribution in space and energy as well as the response of a reactor.

Computer models are used to calculate operational and safety parameters of a reactor core, both before start-up and during operations. These calculations must often be performed in a limited period of time, and computational efficiency is therefore an important consideration. One approach to achieve this efficiency is to use so-called *nodal methods* to numerically solve the diffusion approximation of the neutron transport equation [1]. Nodal methods use average material properties over relatively large regions in the core, and often over broad ranges of incident neutron energy. These material properties are described by cross

sections that are averaged by flux-volume weighting, which results in so-called *few-group homogenized cross sections*.

The homogenized cross sections depend on various thermo-hydraulic and material conditions that may exist in the reactor core. These are known as state parameters. The state parameters that are typically used in PWRs are: burnup, soluble boron concentration, fuel temperature, moderator temperature and moderator density [2].

Two types of homogenized cross sections are used in the full core calculations, namely microscopic and macroscopic cross sections. In this context, a macroscopic cross section is an effective cross section for several isotopes that are lumped together, which also takes into account the number density of each of these isotopes. A microscopic cross section is the probability that a given isotope will undergo a certain reaction, such as absorbing a neutron, averaged over the volume of the homogenized region and weighted by the neutron flux. The older generation of the full core simulators generally utilized macroscopic cross sections. However, there are several advantages of using microscopic homogenized cross sections for some neutronically important isotopes [3] and therefore this model is becoming more prevalent.

The few-group homogenized cross sections are pre-calculated for a limited number of reactor states and represented by mathematical functions in a way that would facilitate their reconstruction at other reactor states during the full core simulation. In the traditional methods, the homogenized cross sections are stored in multi-dimensional tables with either a linear interpolation rule, or a polynomial approximation which is usually limited to second order polynomials [4].

Nodal methods may be less accurate when applied to cores that contain MOX fuel than for cores that are loaded exclusively with UOX fuel [5]. Four ways to increase the accuracy with which both MOX and UOX fuelled cores are modelled are listed in [5], one of which is to increase the number of broad energy groups. A change in the number of broad energy groups may also impact the way in which the cross sections depend on the state parameters in each energy group and therefore the accuracy of a given representation method. The energy group structure that was used in this study is similar to the six-group structure proposed in [6] for modelling some of the important neutron-nuclear interactions for MOX fuelled cores.

The focus of this study is the representation of the few-group homogenized cross sections of a MOX fuel assembly using a sparse grid interpolation method [3, 7, 8], with the aim of limiting the cross section reconstruction errors during full core nodal calculations. This method, which uses a combination of sparse grid sampling and hierarchical polynomial interpolation with Lagrange basis functions, has been successfully applied for the few-group cross section representation of some light water reactors [3, 7, 8].

2. Problem description and methodology

This study addressed the problem of representing a few selected cross sections of a MOX fuel assembly whose specifications are contained in a Nuclear Energy Agency benchmark [9]. A model of this MOX fuel assembly was created in the HEADE (heterogeneous assembly depletion) code [10] of the OSCAR-4 (overall system for calculation of reactors, generation 4) system [11]. Using this model, several sets of the fission, nu-fission, transport and absorption homogenized cross sections were calculated at the sparse grid points in the state parameter space of the MOX fuel.

The homogenized cross sections were calculated for sixteen individual, neutronically important isotopes (namely $^{234}_{92}$U, $^{235}_{92}$U, $^{236}_{92}$U, $^{237}_{92}$U, $^{238}_{92}$U, $^{237}_{93}$Np, $^{239}_{93}$Np, $^{238}_{94}$Pu, $^{239}_{94}$Pu, $^{240}_{94}$Pu, $^{241}_{94}$Pu, $^{242}_{94}$Pu, $^{241}_{95}$Am, $^{135}_{53}$I, $^{135}_{54}$Xe and $^{10}_{5}$B) and two macroscopic cross sections. One of the macroscopic cross sections accounts for the effect of several isotopes lumped together, whilst another accounts for all the remaining isotopes from materials such as cladding and coolant. The homogenized cross sections were calculated using both two and six neutron energy group structures. For the six group cross sections, the group boundaries were set at: $1.10 \cdot 10^{-4}$ eV, $1.40 \cdot 10^{-1}$ eV, $6.25 \cdot 10^{-1}$ eV, 4.00 eV, $5.53 \cdot 10^{3}$ eV, $8.21 \cdot 10^{5}$ eV and $1.96 \cdot 10^{7}$ eV. The boundaries for the two group cross sections were set at $1.10 \cdot 10^{-4}$ eV, $6.25 \cdot 10^{-1}$ eV and $1.96 \cdot 10^{7}$ eV. The boundaries of the state parameter domain were chosen such that the cross section representation is applicable to both day to day reactor calculations and to transient analyses [3]. These intervals are listed in

Table 1. State parameter nominal conditions and boundaries.

State parameter	Nominal	Min	Max
Burnup [MWd/tU]	—	0	60 000
Moderator density [g/cm^3]	0.713	0.313	1.013
Moderator temperature [K]	579.4	279.4	979.4
Fuel temperature [K]	951.4	291.4	1 651.4
Boron concentration [ppm]	600	1	1 600

table 1.

All the cross sections were represented using hierarchical, multi-dimensional Lagrange interpolating polynomials as described in [3, 7, 8]. The interpolation was performed on several sparse grids with an increasing number of sample points in order to investigate how the representation accuracy improves with the number of samples. The representation accuracy can be characterized by the maximum relative error $\delta_{\max}$ and the average relative error δ_{mean}. For practical applications, it is required that these errors do not exceed a specified value that is considered acceptable. In this work, the upper limits for $\delta_{\max}$ and δ_{mean} were set as 0.2 % and 0.05 %, respectively. Although the representation method possesses a built-in way of accuracy assessment, in order to improve the quality of the error characterization, we estimated $\delta_{\max}$ and δ_{mean} using 4 096 independent and uniformly distributed test samples, calculated at the Sobol' quasi-random points [12].

Homogenized cross sections exhibit more complex dependence on some state parameters especially burnup [2]. Therefore in this study, both isotropic and anisotropic sparse grids were used [3, 7, 8]. An isotropic sparse grid contains the same number of samples in all dimensions. Anisotropic sparse grids are formed when any dimension in which the cross section has a prominent dependence is allowed to have more samples in order to improve the accuracy of the representation. The anisotropy of a sparse grid is described by an anisotropy vector $\alpha \in \mathbb{N}^d$, where d is the number of state parameters. The larger the value of the component α_i for a state parameter p_i ($i = 1, \ldots, d$), the smaller the number of points that are sampled for that state parameter. We carried out a study to determine an optimal anisotropic vector that is suitable for the whole library. As a result of the study, the anisotropy vector $\alpha = (1, 2, 2, 2, 2)$ was chosen, where the order of the components corresponds to the order of the state parameters in table 1. This choice of α allows one to have more samples from burnup than from other state parameters.

3. Analysis of the obtained results

Constructing representations of every cross section, reaction type and energy group for all the microscopic and macroscopic materials would result in a library with a total of 152 two-group and 456 six-group cross sections. In this work we constructed representations for a subset of homogenized cross sections, which we considered to be either representative, or playing a prominent role in MOX fuel, or to be the most challenging. For the sake of briefness, the analysis in this paper is limited to three materials: a macroscopic one, which accounts for the effect of several isotopes lumped together, and two microscopic cross sections: $^{239}_{94}$Pu and $^{238}_{92}$U. These materials are important for the operation of a reactor core that contains MOX fuel. For example, the cross sections for the macroscopic material describe the average effect of all the neutron-nuclear interactions that may occur in a reactor core. $^{238}_{92}$U is an important resonance absorber which also has the highest number density of all the isotopes in the fuel. $^{239}_{94}$Pu has the highest number density of all the fissile isotopes in MOX fuel.

Out of all the cross sections represented in our work, we are going to discuss the absorption cross sections. Neutron absorption is an important neutron-nuclear interaction which controls the rate of fission in a thermal reactor. The results will be presented for the thermal neutron energy groups, i.e. groups 5 and

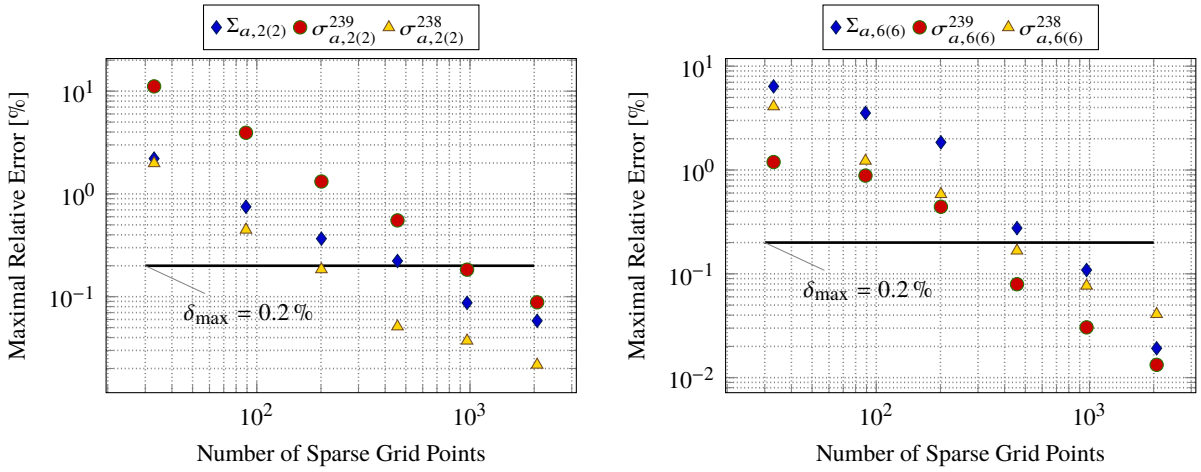

Figure 1. Dependence of the accuracy of the cross section representation on the number of sparse grid points.

6 for the six-group MOX fuel assembly model and group 2 for the two-group model. The boundaries for these groups are within the range in which nuclear fission reactions take place inside a thermal reactor core. We will denote the absorption cross sections for ${}^{239}_{94}$Pu, ${}^{238}_{92}$U and the macroscopic material by $\sigma^{239}_{a,\,g(G)}$, $\sigma^{238}_{a,\,g(G)}$ and $\Sigma_{a,\,g(G)}$ respectively, where $g(G)$ represents the energy group g for the G-group model, e.g. $\sigma^{239}_{a,\,5(6)}$ will be used for the group 5 microscopic cross section for the ${}^{239}_{94}$Pu in six-group model.

Two and six-group absorption cross sections for ${}^{239}_{94}$Pu, ${}^{238}_{92}$U and macroscopic material were interpolated using sparse grids that were constructed hierarchically, using 33, 89, 201, 457, 969 and 2 065 points. The results for the rate at which the maximal relative error, $\delta_{\max}$, decays with the number of sparse grid points[1] are shown in figure 1. As expected, the representation accuracy increases with the number of samples, which means that the method can be used to provide a range of representations, that are optimal in terms of balance between the accuracy and the number of samples.

Table 2 shows the number of samples that are required in order to obtain the target accuracy for each of the three cross sections for all the energy groups in both two- and six-group models. One can see from table 2 that the target accuracy is achieved with less than 1 000 samples in all the cases, which corresponds to a number of transport code runs acceptable in practice. Moreover, one can see that the thermal cross sections require more samples than the fast ones in order to achieve a target accuracy. The number of samples in a sparse grid is connected to the number of basis functions and it reflects the order of the polynomial of the representation function. The high polynomial order indicates the higher complexity of the approximation in terms of its deviation from a constant or linear shape. Therefore, numbers in table 2 demonstrate that the complexity of cross section dependencies increases from fast to thermal groups.

The complexity encountered in the construction of a representation for thermal cross sections is influenced by the degree to which the cross sections vary across the domain. Table 3 shows the magnitude of the percentage variation of the cross sections estimated with 4 096 independent, uniformly distributed test samples, normalized to their median values. In the all cases, one can see that the variation of thermal neutron cross sections is always greater than for the fast neutron cross sections.

As can be seen from figure 1, the representation accuracy for ${}^{238}_{92}$U is smaller when the thermal homogenized cross sections are calculated using a six-group model. This pattern of results also applies to the absorption cross sections for all the neutronically important uranium isotopes. Thus, for uranium isotopes, the two-group cross sections can be approximated with lower order polynomials. This explains

[1] We report and analyze the maximal relative error only because, as our previous studies have demonstrated, it corresponds to the target accuracy, which is more difficult to meet.

Table 2. The number of sparse grid points required to obtain the target representation accuracy.

		Six-group						Two-group	
Energy group		1	2	3	4	5	6	1	2
Cross section	σ_a^{238}	89	33	89	33	457	457	89	201
	σ_a^{239}	89	89	201	89	969	457	89	969
	Σ_a	33	89	89	201	457	969	33	969

Table 3. Variation of the cross sections around the median value, in percent.

		Six-group						Two-group	
Energy group		1	2	3	4	5	6	1	2
Cross section	σ_a^{238}	11.8	1.6	45.0	5.0	21.5	27.2	12.8	30.4
	σ_a^{239}	4.8	0.4	31.6	19.5	56.7	11.8	13.4	120.3
	Σ_a	21.7	10.9	38.5	67.8	61.7	53.2	20.5	72.7

why the traditional methods were successful in representing two-group cross sections for UOX fuel.

One way to explain this shift in complexity is by examining the cross section dependencies on the individual state parameters. This may be achieved by constructing scatter plots from samples (the sparse grid or the independent test set) as a function of each of the five state parameters. Our analysis of such graphs proves that the variation of $\sigma^{238}_{a,\,6(6)}$ is dominated by the non-linear dependence on the burnup and the moderator temperature, while $\sigma^{238}_{a,\,2(2)}$ shows a strong dependence on fuel temperature and moderator density. This observation can be understood by considering that the calculation of the homogenized cross sections involves neutron flux weighting. However, the neutron flux in a reactor core is dependent on the state parameters. Changes in the values of the state parameters affect the neutron distribution in different energy groups differently. These variations result in different values of the neutron flux that are used for the weighting process.

Fewer samples are required to reach the target accuracy for $\sigma^{239}_{a,\,6(6)}$ than for $\sigma^{239}_{a,\,2(2)}$. However, the complexity of representing σ_a^{239} for the other thermal energy group, i.e. group 5, is comparable with that of $\sigma^{239}_{a,\,2(2)}$. This can be understood by considering that the cross section σ_a^{239} has a large resonance in the energy range $1.40 \cdot 10^{-1}$ eV to $6.25 \cdot 10^{-1}$ eV which coincides with group 5 for the six-group model. As a result, $\sigma^{239}_{a,\,5(6)}$ has a higher percentage variation across the state parameter space as compared to $\sigma^{239}_{a,\,6(6)}$. Therefore, for the six-group model, the representation error is isolated into a smaller energy range.

The analysis of thermal reactors that are loaded with MOX fuel can be done with better accuracy if the cross sections are calculated using an energy group structure that removes the complexity of the cross section dependencies away from the energy range in which fission reactions are most likely to take place in plutonium. This is done by increasing the number of energy groups. Whilst an increase in the number of energy groups yields better results for plutonium, this does not hold true for other isotopes. However, the sparse grid method is still capable of representing these cross sections to an acceptable accuracy.

4. Conclusion

The paper addressed the problem of representing a few selected few-group homogenized neutron cross sections of a MOX fuel assembly using the sparse grid method. This method utilizes a combination of

sparse grid sampling and hierarchical polynomial interpolation with multivariate Lagrange basis functions.

In order to improve the efficiency of the cross section representation, a mini-study with a goal to find an optimal (i.e. which can provide the best accuracy for a given number of samples for all cross sections in the library) sparse grid anisotropy vector has been performed. A candidate vector with an equally reduced number of samples for all the state parameters, except the burnup, was identified and used through the rest of this work. Further studies has confirmed that, though different cross sections can exhibit a behavior dominated by different state parameters, the burnup is a state parameter, importance of which is shared by all the homogenized cross sections.

The application of the method to the representation of several two- and six-group cross sections has produced excellent results. Results for the microscopic absorption cross sections for $^{239}_{94}$Pu and $^{238}_{92}$U and for the macroscopic absorption cross sections are reported and analyzed in this paper. The desired representation accuracy, $\delta_{\max} = 0.2\,\%$, was achieved with less than 1 000 samples which make the method suitable for practical application. These results are impressive if we consider that the cross sections used in this work were calculated using intervals of state parameters that are suitable for transient analysis. This means that the cross sections we interpolated have a more complex dependence on the state parameters than the cross sections that are usually used for the normal day-to-day reactor operations.

The primary fissile isotope in MOX fuel, $^{239}_{94}$Pu, poses a problem when the two-group model is used: the accuracy of the representation of its thermal group cross section is exceptionally low. Nevertheless, using the six-group model allows one to palliate the problem by isolating the complexity of the dependence (and the corresponding representation error) in group 5, thus improving the representation accuracy of the sixth group, where the nuclear fission reactions are most likely to take place. This does not address all the limitations of nodal diffusion methods when simulating MOX-fuelled PWR cores, which is an area of study that spans much wider than just cross section representation.

Acknowledgments

The financial assistance of the South African National Research Foundation (NRF) towards this study through an Innovation Master's Scholarship that was awarded to the first author (Grant 89093) and the through Incentive Funding, awarded to the third author (Grant 70730), is hereby acknowledged. Opinions expressed and conclusions arrived at, are those of the authors and are not necessarily to be attributed to the NRF.

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