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Improvements in LFR fuel pin cell calculation by DRAGON5

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ABSTRACT

Deterministic lattice calculations for lead-cooled fast reactors require fine-group cross section libraries, with accurate self-shielding data for both actinides and structural materials. In this work, improvements in library preparation are presented and the libraries are shown to perform well for a LFR fuel pin cell. Two self-shielding methods implemented in DRAGON5, the subgroup method with physical probability tables and Tone's method, are compared against OpenMC reference calculations. A fine 1962-group structure is used, reducing the discrepancy on the multiplication factor by some hundreds pcm with respect to legacy 315-group libraries. Additional self-shielding data for lead isotopes and iron are included, further improving accuracy. Particular attention is paid to the treatment of unresolved resonances, where the standard UNRESR module of NJOY exhibits a behaviour of the dilution-dependent cross sections of ^{239}Pu different from that of the PURR module, which is used to generate a new set of libraries. With the improved libraries, DRAGON5 achieves agreement with OpenMC within 30 pcm on the multiplication factor and sub-percent discrepancies on condensed quantities across most of the energy region of interest. To the autors' knowledge, this is the first published calculation with DRAGON5 which uses libraries specifically created for fast reactor applications.

Keywords: Nuclear reactor physics, Fast-spectrum reactors, Lattice calculation, Resonance self-shielding

1. INTRODUCTION

Deterministic lattice codes are used to solve the Boltzmann equation. The open-source deterministic lattice code chosen for the following calculations is DRAGON5, which has been developed at Polytechnique Montréal for the analysis of thermal reactors, and which offers a variety of flux solution and self-shielding techniques [1]. In recent years, it has been applied to fast reactors [2, 3, 4]. However, the only published article on DRAGON5 about the analysis of Lead-cooled Fast Reactors (LFRs), like those developed by *new*cleo, [5] considers only legacy DRAGON5 libraries for thermal reactors.

Deterministic lattice calculations for fast reactors need cross section libraries with a fine group structure. Particular attention should be drawn to the treatment of the unresolved resonance region (URR), where only statistical data about the resonances in the cross sections are known, since a large portion of the neutron spectrum lies in this energy region. Furthermore, liquid lead applications rely on nuclides whose self-shielding data may not be available in the existing libraries of general lattice transport computer codes [1, 6, 7]. All of this motivates the need for creating dedicated libraries for fast reactor applications.

In this work, new libraries for DRAGON5 are created and their performance is tested on the *new*cleo LFR pin cell with a modified isotopic vector. DRAGON5 calculations based on new libraries are compared against reference calculations obtained with the open-source Monte Carlo code OpenMC version 0.15.1 [8] and the performances of the subgroup method with physical probability tables and Tone's

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method implemented in DRAGON5 are also compared. In Section 2 the theory on which these self-shielding methods are based is explained along with the NJOY2016 [9] calculation scheme used to prepare the libraries. In Section 3, preliminary tests performed to assess the performance of a fine group library against a broad group one, the effect of lead self-shielding and the improvements obtained with a different method to calculate self-shielding data in the URR are shown. Finally, some results for the pin cell are presented. All the calculations presented were performed on a workstation and parallelised on 8 threads.

2. THEORY AND METHODOLOGY

2.1. Self-Shielding Methods

Resonance self-shielding is the presence of depressions in the neutron flux at energies corresponding to resonances in cross sections of different isotopes. Correct treatment of this phenomenon is necessary to obtain an accurate calculation and is particularly important for LFRs since the cross sections of the isotopes in the coolant of these reactors have resonances, a key difference from water-cooled reactors.

2.1.1. Subgroup method with physical probability tables

Subgroup methods are based on discretised Lebesgue integrations using quadratures named "probability tables" [10]. Each energy group is subdivided into N subgroups, each of them corresponding to a base point σ_k, which is the value of the total cross section in the subgroup. A probability table is a list of couples (σ_k, P_k), where P_k is the probability relative to σ_k. Dilutions quantify the effect of non-resonant isotopes on the self-shielding of the resonant absorber and is defined by NJOY as $\sigma_d = \Sigma^\dagger / N^*$, where $\Sigma^\dagger$ is the total macroscopic cross section of non-resonant isotopes and N^* is the atomic density of the resonant one. The SUBG approximation of DRAGON5 [11] consists in computing probability tables in such a way that the cross section at any dilution is interpolated as

$$\bar{\sigma}(\sigma_d) = \left\langle \frac{\sigma}{\sigma + \sigma_d} \right\rangle_g \Bigg/ \left\langle \frac{1}{\sigma + \sigma_d} \right\rangle_g = \sum_{k=1}^{N} \frac{P_k \sigma_k}{\sigma_k + \sigma_d} \Bigg/ \sum_{k=1}^{N} \frac{P_k}{\sigma_k + \sigma_d} , \tag{1}$$

so that the infinite-dilution microscopic total cross section is $\bar{\sigma}(\infty) = \sum P_k \sigma_k$. In DRAGON5, self-shielding calculations can be performed for many isotopes, but each one is treated separately in a process called "Bondarenko iterations" in which the other resonant isotopes are approximated as non-resonant, iterating until convergence.

The collision-probability (CP) formulation of the self-shielding treatment begins by considering the CP form of the slowing-down equation in every region i and subgroup k:

$$\phi_{i,k} = \sum_{j=1}^{I} p_{ij,k} \left[\Sigma^\dagger_{s,j} + N^*_j \left(\lambda_g \sum_{\ell=1}^{N} P_\ell \sigma^*_{s,j,\ell} \phi_{j,\ell} + (1 - \lambda_g) \sigma^*_{s,j,k} \phi_{j,k} \right) \right] , \tag{2}$$

where $p_{ij,k}$ is the reduced collision probability for the k-th subgroup, $\Sigma^\dagger_{s,j}$ is the macroscopic P_0 scattering cross section for non-resonant isotopes in the j-th region, N^*_j is the atomic density of the resonant isotope in the j-th region, $\sigma^*_{s,j,k}$ is the microscopic P_0 scattering cross section for the resonant isotope, the index ℓ runs on the subgroups and λ_g is the Goldstein-Cohen parameter, whose values are bounded between 0 and 1, values corresponding to wide resonance and statistical approximations. Equation (2) can be solved iteratively until convergence of the subgroup flux unknowns. Then, the probability tables are used to calculate the integrated flux and reaction rates for the resonant isotope in each group g and

region i for the ρ-th interaction as:

$$\langle \phi_i \rangle_g = \sum_{k=1}^{N} P_k \phi_{i,k}, \qquad \langle \sigma_{\rho,i} \phi_i \rangle_g = \sum_{k=1}^{N} P_k \sigma_{\rho,i,k} \phi_{i,k} \, . \tag{3}$$

These quantities are then used to compute the microscopic cross section as $\sigma_{\rho,g} = \mu_g \langle \sigma_{\rho,i} \phi_i \rangle_g / \langle \phi_i \rangle_g$ where μ_g is the superhomogenisation factor [11] which is needed to preserve the reaction rates when heterogeneous geometries are considered.

2.1.2. Tone's method

Tone's method [12] is based on a homogeneous-heterogeneous equivalence procedure. Its derivation starts from the collision probability form of the Boltzmann equation for a generic slowing-down kernel $\mathcal{R}_j^*\{\phi_j(u)\}$ for the resonant isotope and in the j-th region of the geometry

$$\phi_i(u) = \sum_{j=1}^{I} p_{ij}(u) \left(\Sigma_j^\dagger + \mathcal{R}_j^*\{\phi_j(u)\} \right) \, , \tag{4}$$

where $\Sigma_j^\dagger$ is the macroscopic total cross section of the non-resonant isotopes in the j-th region. The main assumption of Tone's method is that $P_{ji}(u) = \alpha_i(u) P_{ji,g}$, meaning that the fine lethargy dependence of the collision probabilities in each energy group depends only on the arrival region i and where $\alpha_i(u)$ is the Tone lethargy function. A lengthy derivation using reciprocity and conservation relations of collision probabilities then shows that

$$\phi_i(u) = \frac{\mathcal{R}_i^*\{\phi_i(u)\}/N_i^* + \sigma_{d,g,i}}{\sigma^*(u) + \sigma_{d,g,i}} \, ; \qquad \sigma_{d,g,i} = \sum_{j=1}^{I} V_j P_{ji,g} \Sigma_j^\dagger \Big/ \sum_{j \in G_x} V_j P_{ji,g} N_j^* \, , \tag{5}$$

where $\sigma_{d,g,i}$ is the equivalent dilution in the g-th group and i-th region and G_x is the set of indices pointing to resonant regions.

The direct self-shielded cross sections $\hat{\sigma}_{\rho,i,g}$ are obtained by interpolating the equivalent dilution $\sigma_{d,i,g}$ with the cross section tables computed by NJOY for each group. In DRAGON5, direct self-shielded cross sections undergo a superhomogenisation correction $\tilde{\sigma}_{\rho,i,g} = \mu_{i,g} \hat{\sigma}_{\rho,i,g}$ similar to that performed in Section 2.1.1 in order to preserve the reaction rates.

2.2. Library Production with NJOY

DRAGON5 runs require nuclear data libraries in the so-called DRAGLIB format which contain all the data needed for the calculations, including cross sections in a multigroup structure. In this work, they were created with the nuclear data processing code NJOY2016, supplemented by a module called DRAGR for formatting multigroup data. NJOY processes data from evaluated nuclear data libraries, reconstructing cross sections, applying thermal broadening, and evaluating heat production and dilution dependent cross sections if needed. DRAGR then takes the output data of NJOY and creates a DRAGLIB library. All libraries in this work were created from ENDF/B-VIII.0 [13] evaluated libraries.

To allow for self-shielding with physical probability tables and Tone's method, one needs dilution-dependent cross sections which are evaluated in the GROUPR module of NJOY. In this module, the so-called flux calculator was used for all energies, as it includes more precise information on transport.

Dilution-dependent cross sections were only included for actinides, lead isotopes and ^{56}Fe in this work, and care was taken to choose parameters in the DRAGR module so that all energy groups with resonances, both resolved and unresolved, included dilution dependence. To calculate dilution dependence

in the URR, either the module UNRESR or PURR were used. While UNRESR is typically used for libraries with deterministic codes and PURR is used to create Levitt-type probability tables in Monte Carlo codes, both produce information that can be used to evaluate dilution dependence in a group structure with GROUPR.

3. PREPARATION AND TESTING OF LIBRARIES FOR DRAGON5

3.1. Fine Group Structure Testing

This study was performed considering a fuel pin cell representative of the LFR-AS-200 developed at *new*cleo. A group structure containing 1962 energy groups was used, and three libraries with different data content based on this group structure were prepared through this work, as listed in Table I. The group structure is identical to that of ECCO-1968 [14], except that group boundaries that break the constant lethargy width of groups in the fast region are removed. The lethargy width chosen comes from the scattering reactions off actinides which give the lowest lethargy gains. Specifically, it is chosen as the average lethargy gain in scattering off ^{238}U. Neutron scattering in lead exhibits a similar lethargy gain and does not significantly alter this assumption. Instead, libraries for thermal reactors can be based on broad groups because scattering in water leads to a high lethargy gain and few events thermalise neutrons.

The DRAGON5 1962-NOPbSS library was prepared with this fine group structure and compared with the legacy DRAGON5 SHEM-315 library meant for thermal reactor analysis that contains the same isotopic data. In this calculation, the self-shielding treatment was applied to actinides and ^{56}Fe. In this work, the results obtained from DRAGON5 are compared against OpenMC references considering $\Delta k_\infty = k_\infty^{\text{DRAGON5}} - k_\infty^{\text{OpenMC}}$ for the multiplication factor and the relative discrepancy $\varepsilon_g = X_g^{\text{DRAGON5}} / X_g^{\text{OpenMC}} - 1$ for quantities condensed in 33 groups such as fluxes and cross sections, where the g subscripts denote the energy group. As shown by the data in Table II and Figure 1a, the new library performs better than the legacy one, with a reduction of the discrepancy on the multiplication factor of around 250 pcm for both self-shielding methods. Since 98% of the neutron flux lies in the energy region between 300 eV and 6 MeV, only this region was considered for the analysis of quantities condensed in 33 groups. Relative discrepancies are small at high energy, but start to increase at energies below 40 keV. The increase in the number of energy groups leads to an increase in the runtime from ∼15 s of the SHEM-315 to ∼110 s of the 1962-NOPbSS.

Table I. Summary of the libraries used in the presented calculations.

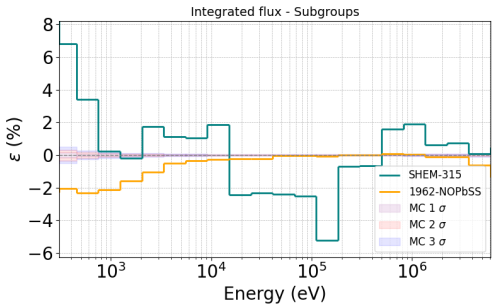
Name	# groups	Pb self-shielding	NJOY module
SHEM-315	315	No	UNRESR
1962-NOPbSS	1962	No	UNRESR
1962-UNRESR	1962	Yes	UNRESR
1962-PURR	1962	Yes	PURR

3.2. Data addition to library

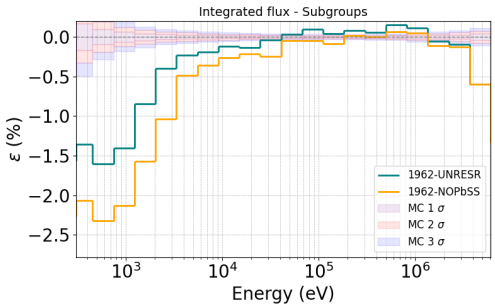
Despite the 1962-group structure results in a substantially lower value for Δk_∞, the calculation can still be improved by applying the self-shielding treatment to lead. Moreover, iron should undergo the self-shielding treatment in an energy range wider than the one previously considered. Both these considerations are needed because these isotopes have resonances at the energy where the fast-neutron flux is concentrated. Therefore, the 1962-NOPbSS library was further refined into the 1962-UNRESR

Table II. Δk_∞ comparison for different cases.

Options	k_∞	Δk_∞ (pcm)
Subgroup SHEM-315	1.27975	-459
Subgroup 1962-NOPbSS	1.28218	-216
Subgroup 1962-UNRESR	1.28439	-44
Subgroup 1962-PURR	1.28423	-11
Tone 1962-PURR	1.28411	-23
OpenMC	1.28434 ± 6 pcm	



(a) Comparison between the SHEM-315 and the 1962-NOPbSS libraries.



(b) Comparison between the 1962-NOPbSS and the 1962-UNRESR libraries.

Figure 1. Relative discrepancies with respect to OpenMC for fluxes integrated over volume and energy condensed in 33 groups.

library by adding self-shielding data for lead isotopes and ^{56}Fe up to 6 MeV. Consequentially, the calculations in which these isotopes underwent a self-shielding treatment were compared against the old one, where self-shielding was applied only to fuel isotopes. The results for the multiplication factor are presented in Table II and the relative discrepancies of the integrated fluxes are shown in Figure 1b. The multiplication factor discrepancy is reduced by ∼170 pcm for both self-shielding methods and the discrepancy for the integrated flux condensed in 33 groups is also improved at any energy, but it is high at energy below 40 keV.

3.3. New Library Production Method

Since the studied pin cell has a fast spectrum, a large portion of the neutron flux lies in the URR. Therefore, an in-depth analysis of the discrepancy in the URR was conducted. As shown in Figure 3, the relative discrepancies increase in that region and may arise from an improper treatment of the unresolved resonances. Thus, the new 1962-PURR library was prepared by treating the URR with the PURR module of NJOY instead of the UNRESR module, and the dilution-dependent cross sections of these two libraries were compared. As depicted in Figure 2, they have dramatically different functional forms. The key difference between these modules is that PURR samples resonance statistically, while UNRESR integrates over the probability distribution for resonances, applying a series of approximations [9]. If the statistical sampling in PURR is performed on a sufficiently fine ladder, the calculations are more precise than those of UNRESR. In OpenMC, the URR is treated with Levitt-type probability tables.

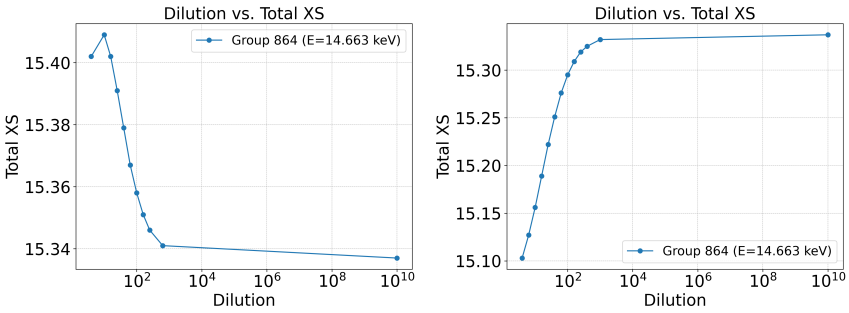


Figure 2. Dilution-dependent cross section of ^{239}Pu in an energy group in the unresolved resonance region. Left and right curves correspond to UNRESR and PURR, respectively.

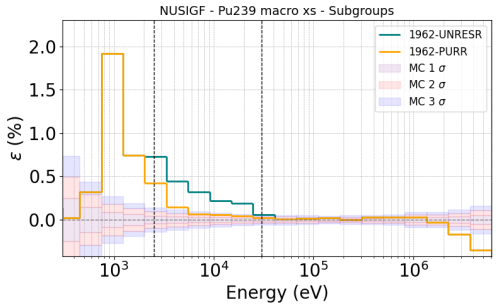


Figure 3. Comparison of relative discrepancies with respect to OpenMC for the $\nu\Sigma_f$ macroscopic cross section of ^{239}Pu condensed in 33 groups for the 1962-UNRESR and the 1962-PURR libraries. The vertical lines show the boundaries of the unresolved resonance region of ^{239}Pu.

3.4. Final Pin Cell Results

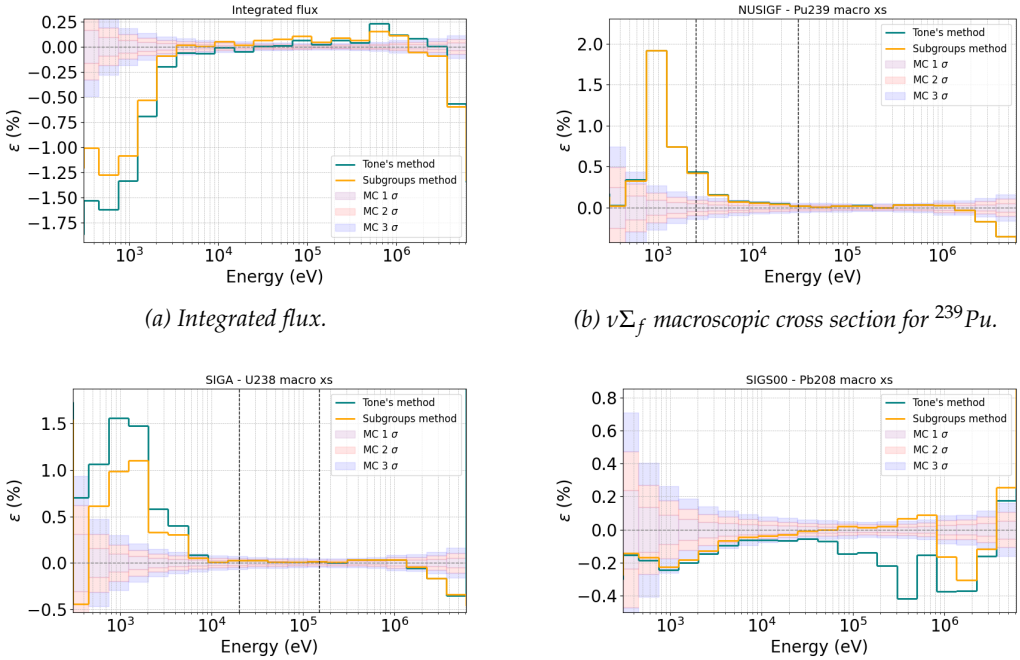
A DRAGON5 calculation was performed on the pin cell using the 1962-PURR library. Figure 3 shows the difference in the quality of the calculations in the URR resulting from the module used to prepare the dilution-dependent cross sections in this region. This results in a significant improvement of the calculation of the multiplication factor, as presented in Table II, with discrepancies in the order of 30 pcm. Quantities condensed in 33 groups are also calculated with higher precision, as shown in Figures 4a to 4d, with discrepancies smaller than 1% in most of the energy region of interest. Some discrepancies are still present at low energies, and may arise from some resonant isotopes in the cladding and in the coolant that did not undergo any self-shielding treatment. With this new libraries, one-group condensed criticality factors and their relative discrepancies with respect to the OpenMC reference were computed. As presented in Tables III and IV, the subgroup method gives better results than Tone's method for each calculated quantity. Taking into account CPU fluctuations, the computational performance of the two methods is equivalent, fluctuating around 115 s.

Table III. 1962-PURR library criticality factors.

Options	η	ε_η	f	ε_f	Σ_{tr} (cm^{-1})	$\varepsilon_{\Sigma_{tr}}$
Tone	1.3331	-0.09%	0.9591	-0.10%	0.30006	-0.32%
Subgroup	1.3335	-0.06%	0.9600	-0.01%	0.30064	-0.13%
OpenMC	1.3342 ± 10 pcm		0.9601 ± 10 pcm		0.30101 ± 3 pcm	

Table IV. 1962-PURR library 1-group condensed macroscopic cross sections.

Options	$\nu\Sigma_f^{^{239}Pu}$ (cm^{-1})	$\varepsilon_{\nu\Sigma_f^{^{239}Pu}}$	$\Sigma_a^{^{238}U}$ (cm^{-1})	$\varepsilon_{\Sigma_a^{^{238}U}}$	$\Sigma_{s,0}^{^{208}Pb}$ (cm^{-1})	$\varepsilon_{\Sigma_{s,0}^{^{208}Pb}}$
Tone	0.0039114	0.03%	0.0019204	0.08%	0.067916	-0.17%
Subgroup	0.0039116	0.03%	0.0019190	0.01%	0.068020	-0.01%
OpenMC	0.0039103 ± 0.04 pcm		0.0019188 ± 0.02 pcm		0.068028 ± 0.7 pcm	



(a) Integrated flux.

(b) $\nu\Sigma_f$ macroscopic cross section for ^{239}Pu.

(c) Σ_a macroscopic cross section for ^{238}U.

(d) $\Sigma_{s,0}$ macroscopic cross section for ^{208}Pb.

Figure 4. Relative discrepancies with respect to OpenMC for quantities condensed in 33 groups for the 1962-PURR library.

4. CONCLUSIONS

A new method for the preparation of deterministic libraries was proposed to improve the quality of pin cell calculations with DRAGON5. A new 1962-PURR library was prepared in order to apply self-shielding treatment to actinides, lead and ^{56}Fe, resulting in a Δk_∞ with respect to the OpenMC reference of 11 pcm with the subgroup method with physical probability tables and one of 23 pcm with Tone's method. Compared to the legacy SHEM-315 library, this new library led to a reduction of around 450 pcm in the discrepancy in k_∞ with respect to the OpenMC reference. The quality of results condensed in 33 groups improved accordingly, with relative discrepancies smaller than 2% in the energy region with the largest portion of the neutron flux. Criticality factors and macroscopic cross sections condensed in one group were found to have relative discrepancies below 0.35% with respect to the OpenMC reference.

A major result of this work is the importance of lead self-shielding in LFR applications, along with the confirmation of the importance of fine-group structures for fast-spectrum applications. Additionally, the quality of calculations in the URR were found by using the PURR module of NJOY rather that

the UNRESR module. Two different self-shielding modules in DRAGON5 were compared, with results obtained with the subgroup method found to be slightly better than those of Tone's method. This observation may be explained by the additional information included into probability tables and used only by the subgroup method. Additional justifications will be included in the forthcoming investigations. In general, these results highlight the importance of adopting tailored group structures and resonance treatments to achieve accurate deterministic lattice calculations for LFR fuel pin cells. Further improvements of the quality of the calculation can be obtained with a study of the sources of discrepancies in the resolved resonance region, and future work should also consider other pin cells, assemblies and full-core calculations.

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