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APPLICATION OF ADVANCED SELF-SHIELDING MODELS TO CRITICALITY-SAFETY STUDIES

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ABSTRACT

Recent improvements made in resonance self-shielding algorithms for reactor physics calculations can certainly be applied to criticality-safety studies. In this paper we investigate the possibility of using resonance self-shielding models based on the subgroup approach, conjointly with innovative energy meshes such as SHEM extended to 295 and 361 energy groups, to generate sets of homogenized, self-shielded, macroscopic cross sections. These group constants are then used in a multigroup Monte Carlo calculation. To do so, the lattice code DRAGON has been combined with the Monte Carlo code MORET, using experimental benchmarks from ICSBEP as a framework for validation. Numerical results show great concordance with experimental values and those of others, well validated, criticality codes.

Key Words: Criticality-Safety, Resonance self-shielding, Lattice code DRAGON, Monte Carlo code MORET, ICSBEP.

1. INTRODUCTION

In criticality-safety, the main objective is to determine the risk of an ungoverned start of a chain reaction in a system containing fissile materials. A macroscopic indicator of criticality is the k_{eff}, defined as the effective multiplication factor of the neutronic population. Most criticality-safety code packages currently provide three ways for evaluating the k_{eff} of a given system:

- A purely stochastic: a Monte Carlo calculation is performed using pointwise cross sections on the detailed geometry.
- A full deterministic way, in which multigroup, self-shielded cross sections provided by a lattice code can be collapsed to a few energy groups. Usually, a discrete ordinates (S_N) method is next applied on an simplified geometry using these cross sections, resulting in a straightforward, albeit sometimes crude, evaluation of the k_{eff} of the system.
- A coupled deterministic/Monte Carlo way: a lattice code generates multigroup, self-shielded, spatially homogenized cross sections. A 3D multigroup Monte Carlo

calculation is then performed using these group-constant cross sections, leading to an important CPU time saving. Examples of Monte Carlo multigroup criticality programs widely used are MORET4 [1] in the CRISTAL [2] system, or KENO6 [3] in the SCALE [4] software.

From an industrial viewpoint, a systematic use of a Monte Carlo calculation with pointwise cross sections could be prohibitive, due to its huge calculation time. On the other hand, geometrical approximations done during the full deterministic way can lead to relatively misleading errors. Furthermore, the use of multigroup, spatially homogenized cross sections in a 3D Monte Carlo calculation can lead to acceptable results in most of encountered configurations. Thus, the multigroup Monte Carlo approach is daily used for criticality-safety studies, both for design or operating studies.
The generation of group constants, needed as input by the Monte Carlo code, and most notably the resonance self-shielding method is a good candidate to improvements. While in the SCALE package, resonance self-shielding calculations are usually based on the classical Bondarenko method [5] or on the Nordheim method [6], a new module makes possible the determination of self-shielded multigroup cross sections using a very fine energy mesh [7]. Regarding the APOLLO2-MORET4 scheme in the CRISTAL code, the self-shielding operator relies on the use of probability tables but is not typically a subgroup method, as an equivalent dilution is computed for each resonant isotope in each resonant group and serves as an interpolation variable for determining the effective cross section [8]. Moreover, applied slowing-down models depend on the neutronic spectrum and on present isotopes. In this proposed work, different self-shielding algorithms based on the subgroup method have been confronted to criticality-safety calculations. The lattice code DRAGON [9] feeds the Monte Carlo code MORET with sets of self-shielded, homogenized cross sections. Thanks to its large representativeness in term of encountered isotopes and spectral configurations, criticality benchmarks such as ICSBEP [10] represent a powerful tool for experimental validation.

2. THE MULTIGROUP MONTE CARLO APPROACH

2.1. Generation of constant cross sections

A multigroup Monte Carlo approach requires a homogenized and self-shielded cross section library. This library can be generated by a lattice code, such as DRAGON, or by a collection of independent modules, as it is done for instance in the SCALE package. Lattice calculation involves a geometrical approximation: each part of the system is considered independently, using either an infinite, homogeneous representation or an infinite lattice (usually 1D or 2D) modeling. A resonance self-shielding calculation is then mandatory in order to take into account the local depression of the fluxes, due to resonant behavior of cross sections in each energy group. Thus, a neutron flux calculation can be performed on the consistent multigroup representation of the neutron energies (typically between 50 and 400 groups are used). Next, the integrated fluxes and reaction rates corresponding to different partial cross sections are obtained, and direct weighted cross sections (flux-volume weighting) are computed, leading to a set of constant cross sections that can be used as input in the multigroup Monte Carlo code. In case of non-homogeneous output geometries, a *superhomogenization* (SPH) equivalence procedure can be applied in order to force the preservation of reaction rates [11]. Fig. 2 illustrates the computational approach used

in the lattice code DRAGON to generate problem dependent multigroup cross sections for typical criticality-safety studies. These self-shielded, homogenized cross sections can then serve as input library for a multigroup Monte Carlo evaluation of the K-effective on the 3D geometry.

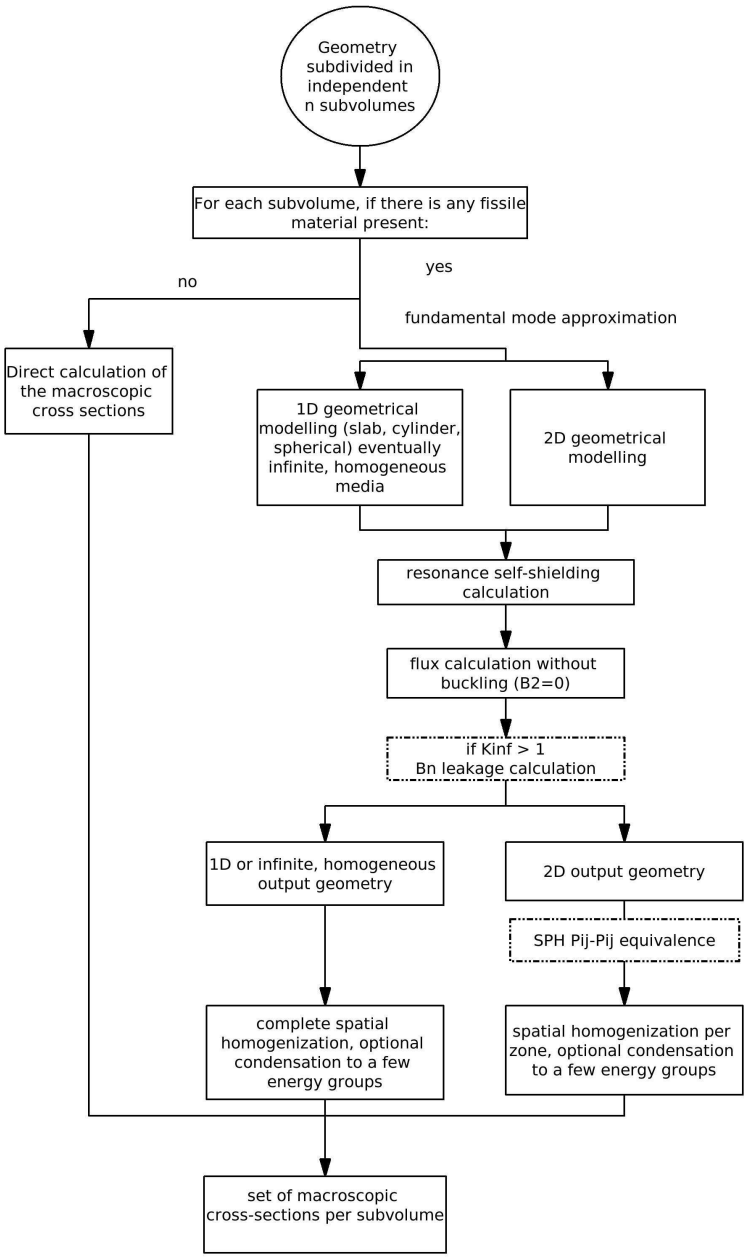

Figure 1. Generation of macroscopic cross sections per region by a DRAGON lattice calculation

2.2. Self-shielding calculations: the subgroup approach

Regarding the resonance self-shielding calculations, different classes of methods are available in the lattice code DRAGON. The module `SHI:` was developed first and relies on rational expansions of fuel-to-fuel collision probabilities [12].
In this study, we have particularly emphasized the methods relying on the subgroup approach as implemented in the `USS:` module. In this approach, the detailed energy-dependent cross section behavior is replaced by its probability density representation $\Pi(\sigma)$ in each coarse energy group, in such a way that $\Pi(\sigma)d\sigma$ is the probability for σ to have its value between σ and $\sigma + d\sigma$. Using this definition, any Riemann integral in lethargy with a σ-dependent integrand can then be rewritten with an equivalent Lebesgue integral

$$\frac{1}{\Delta u_g}\int_{u_{g-1}}^{u_g} du f[\sigma(u)] = \int_0^{max(\sigma)} d\sigma \Pi(\sigma) f(\sigma) \tag{1}$$

The discretization of these probability densities leads to quadrature sets called probability tables

$$\Pi(\sigma) \simeq \sum_{k=1}^{K} \delta(\sigma - \sigma_k)\omega_k, \tag{2}$$

Replacement of 2 in 1 leads to

$$\frac{1}{\Delta u_g}\int_{u_{g-1}}^{u_g} du f[\sigma(u)] \simeq \sum_{k=1}^{K} \omega_k f(\sigma_k) \tag{3}$$

The resulting quadrature $\{\omega_k, \sigma_k\}_{k\in[1,K]}$ is the probability table for the variable σ in group g. These probability tables are finally used within the flux solution algorithm of the subgroup method. Several computational approches exist for the determination of these probability tables, leading to different classes of subgroup methods.
A major drawback of the subgroup approach relies on the fact that in the slowing-down domain, the correlations existing between the resonances in the main collision term in the transport equation and those in the scattering operator are neglected. To take this correlation into account, different approaches have been adopted, and in its study three classes of subgroup models have been confronted to criticality calculations:

- The statistical subgroup model (USS), relying on physical probability tables. In this case, the probability table components are obtained by performing a root-mean-square (rms) fit over a set of dilution-dependent cross sections [18].
- The Ribon extended model (PTSL), depending on the use of mathematical probability tables. This approach is an extension of the CALENDF formalism, with the calculation of mathematical probability table components of the elastic slowing-down operator [18].
- The subgroup projection method (SPM), used only with optimized energy meshes such as SHEM-295g or SHEM-361g. This model is a straightforward simplification of the Ribon extended method, without discretization of the slowing-down equations. This is possible using a very fine energy mesh in the slowing-down range [16].

All these methods permit the representation of *spatially distributed* self-shielding effects. The Ribon extented model and the subgroup projection method also have the possibility to take into account *mutual* self-shielding effects. However, note that we have used these capabilities only for 2D-lattice calculations, as it is not required for legacy criticality studies in which infinite homogeneous or 1D infinite lattice representations are assumed to be sufficiently accurate.

2.3. k_{eff} calculation

In this step, two kinds of criticality calculations can be done. Usually, the Monte Carlo MORET code uses as input the multigroup, self-shielded cross sections and evaluates the k_{eff} of the system with a realistic 3D modeling of the geometry. In another way, a discrete ordinates method can be applied on a simplified geometry, using cross sections collapsed to a few groups of energy (typically 26 groups are used). This method has been established as very accurate, so far as the regular, orthogonal geometrical approximations made in the S_N solution remain applicable.

3. NUMERICAL RESULTS

Some critical experiment benchmarks have been picked up from the ICSBEP handbook for their similarities with industrial studies. Besides, we have chosen a sample of configurations representative of the entire energy spectra. These experiences have been modelized, and comparison between computed and experimental k_{eff} are provided in the next paragraphs.
A preliminary study is presented using for both lattice codes DRAGON and APOLLO2 and the same input library, in order to mitigate the effect due to the processing of the cross sections with distinct options or even versions of NJOY. This enables us to underline directly the influence of self-shielding operators. Regarding the APOLLO2-MORET4 calculations performed in the framework of the CRISTAL package, some explanations of discrepancies between computed and experimental values can be found in [14].

In a second part, the use of DRAGLIB libraries in criticality-safety studies have been thoroughly tested on several ICSBEP benchmarks. Notably, the use of energy meshes such as SHEM-281 [15] and SHEM extented to 295 [16] and 361 [17] groups have been experimented. Self-shielding operators denoted respectively as USS, PTSL and PT can be summarized as follow:

- USS: physical probability tables are employed for *all resonant groups* as described in Ref [18]. A statistical (ST) slowing-down model is set in most of these groups and a wide-resonance (WR) model is set in a few low-energy groups.
- PTSL: Depending on the energy mesh, the Ribon extented model is set:
  - between 2.76 eV and 677.28 eV in the XMAS 172-group,
  - between 22.53 eV and 748.51 eV in the SHEM 281-group.
- For the PT operator, CALENDF-type probability tables are now available:
  - between 4.63 eV and 1113.7 eV in the SHEM 295-group,
  - between 22.53 eV and 1113.7 eV in the SHEM 361-group.

For both PTSL and PT operators, physical probability tables with a statistical (ST) slowing-down model are used in the unresolved part of the spectrum.

3.1. MIX-MISC-THERM-001: influence of the self-shielding approach

This experience corresponds to UO_2-PuO_2 array of pins in U-Pu nitrate solutions. Neutronic spectrum of these configurations is in the thermal part of the energy domain. These cases are typical of fuel pins dissolution during the recycling, and have the particularity to present fissile materials both in pins and in solutions.
We first present a direct comparison of the APOLLO2-MORET4 and DRAGON4-MORET4 numerical results. In order to emphasize the impact of the self-shielding operators in both codes, the same microscopic isotopic data is used in input, i.e. the 172-group CEA93v6 library based on the JEF2.2 evaluation. The self-shielding operator in the APOLLO2 lattice code relies on the Sanchez-Coste model (matrix dilution approach) and the infinite mass approximation. The difference between computed and experimental values is confronted to the uncertainty margin defined as

$$3\overline{\sigma} = 3\sqrt{\sigma^2_{MORET} + \left(\frac{\delta k^{exp}_{eff}}{3}\right)^2}$$

Discrepancies in pcm between experimental and numerical k_{eff} are evaluated for three self-shielding operators available in the lattice code DRAGON (SHI, USS, PTSL), and for the lattice code APOLLO2 (A2), using $C - E = \left(k^{calc}_{eff} - k^{exp}_{eff}\right)$.

Exp. ($k_{eff} \pm \delta k^{exp}_{eff}$)	SHI (pcm)	USS (pcm)	PTSL (pcm)	A2 (pcm)	$3\overline{\sigma}$ (pcm)
1 (1.0000±0.00440)	-177	-587	-835	-453	450
2 (1.0000±0.00440)	429	10	-316	213	450
3 (1.0000±0.00440)	289	-84	83	236	450
4 (1.0000±0.00440)	-160	-442	333	-304	450
5 (1.0000±0.00440)	688	270	449	382	450
6 (1.0000±0.00320)	688	312	-87	447	333
7 (1.0000±0.00320)	451	266	-166	254	333
8 (1.0000±0.00320)	435	233	-178	275	333
9 (1.0000±0.00660)	475	49	274	256	666
10 (1.0000±0.00660)	410	257	448	351	666
11 (1.0000±0.00250)	1374	1261	1072	2418	265
$\overline{\epsilon}$(mean error)	445	150	98	370	450

Table I. DRAGON/APOLLO2 Comparizon using CEA93v6 as input library

Numerical results clearly show the ability of subgroup based self-shielding operators USS and PTSL to handle criticality-safety analysis. Moreover, the Stamm'ler method as available in the lattice code DRAGON in the `SHI:` module, remains acceptable in comparison with the uncertainty margins. Note also that experimental value of case 11 is known to be doubtful.

Reference Monte Carlo calculations using pointwise cross sections confirm this incoherent behavior.

3.2. Use of DRAGLIB library

One of the main objectives of this work was to achieve a good level of accuracy using the PyNJOY system, enabling the construction of DRAGLIB type cross section libraries by interfacing NJOY99 with an additional module, DRAGR [19]. Cross-sections libraries are then built from scratch with NJOY release 99.259+upnea027 [20], using the ENDFB7r0 data library. Comparison between APOLLO2-MORET solutions are also provided, keeping in mind that APOLIB input libraries are built from the JEF2.2 evaluation. A few results are presented here, as more than 300 experiences have been modelized.

3.2.1. Influence of SHEM-extended energy meshes

- HEU-SOL-THERM-001
  This experience involves high-enriched UO_2 solutions and is representative of different fuel cycle configurations (fabrication, dissolutions...).

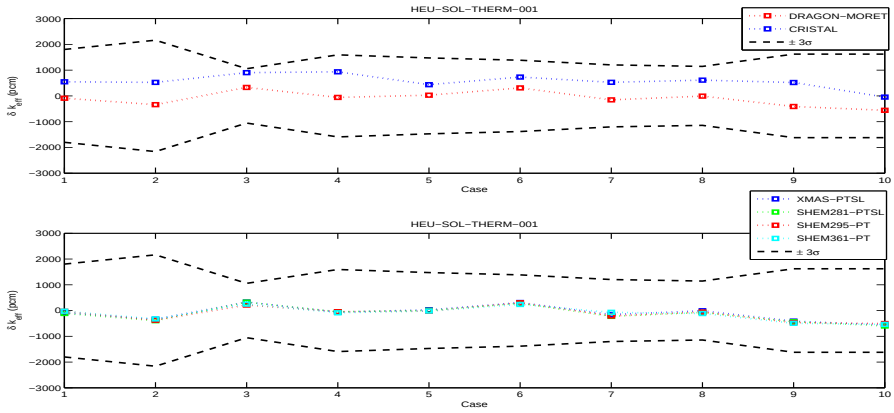

Figure 2. HEU-SOL-THERM-001

- LEU-COMP-THERM-033
  This experience is a modelization of low enriched uranium-oxyde array of pins, with a neutronic spectrum in the thermal energy range.

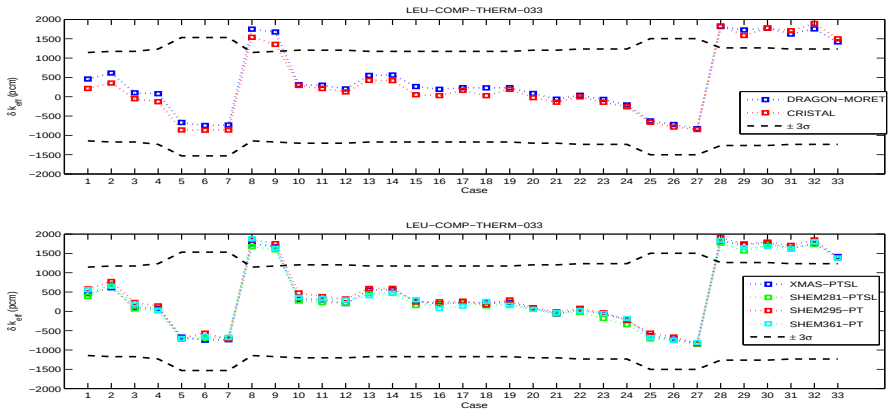

Figure 3. LEU-COMP-THERM-033

- MIX-COMP-THERM-012
  This benchmark represents array of boxes of highly enriched U+Pu powders.

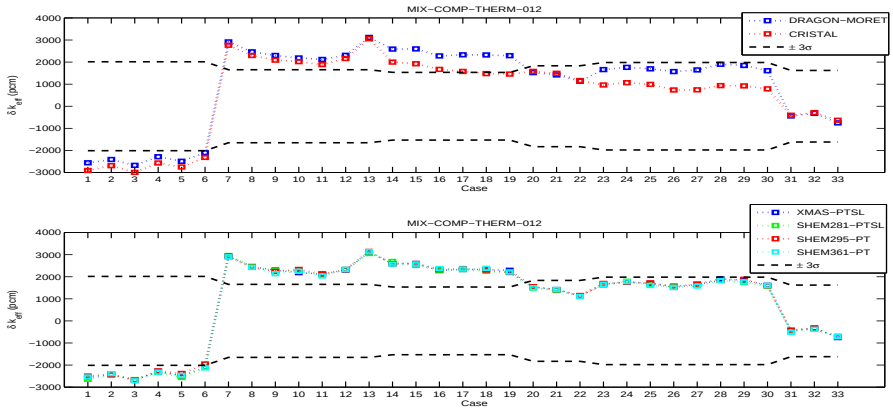

Figure 4. MIX-COMP-THERM-012

To summarize, numerical results show concordance between :

- APOLLO2-MORET results with the CEA93v6 library and DRAGON-MORET with the DRAGLIB input library.
- the different self-shielding operators and energy grids in the lattice code DRAGON:
  - XMAS 172-group and SHEM 281-group with the Ribon extented formalism (PTSL).
  - SHEM 295-group and SHEM 361-group with the subgroup projected method (PT).

3.2.2. LEU-COMP-THERM-041: 3D Monte Carlo vs. S_N 2D calculation

This case illustrates the possibility to replace the 3D Monte Carlo simulation by a 2D or 3D S_N calculation. LEU-COMP-THERM-041 represents low-enriched, UO_2 pins as in PWR assemblies stocked in pool, for which a 2D modelization has been used in the lattice code DRAGON. Besides, these cases present strong localized flux variations and a 1D representation is innapropriate to compute self-shielded, homogenized cross sections.

Group-constant cross sections are generated using a collision probability method on the exact geometry of the assembly. A SPH procedure is mandatory in this case, to force the conservation of the reaction rates. Distributed self-shielding effects are taken into account by splitting each pin into six rings. Then, two possiblities are given, typically either the S_N solver [21] of the lattice code DRAGON or the Monte Carlo code MORET performs the eigenvalue calculation. Both S_N and Monte Carlo use in input the same information, i.e., macroscopic cross sections generated respectively by

- a method of characteristics (MOC),
- a collision probability (CP) method,
- an interface-current method ($J_{\pm}$).

Regarding S_N calculations, parametric studies established that parabolic Diamond-Differencing spatial scheme and a S_{16} level-symmetric angular quadrature are sufficiently accurate. Anisotropy of the scattering cross sections is taken into account up to P_5 order for all isotopes. A JEF2.2 based DRAGLIB library is used as input, with an XMAS-172 group.

Case	Solver	k_∞ D4(USS)-M4	C-E	k_∞ D4(USS)-S_N	C-E
1 (1.1990±0.0062)	MOC	1.20182 ±0.0003	282	1.20187	287
	CP	1.20084 ±0.0003	184	1.20187	287
	$J \pm (DP_1)$	1.20170 ±0.0003	270	1.21318	1418
2 (1.1060±0.0062)	MOC	1.10161 ±0.0003	-439	1.10302	-298
	CP	1.10100 ±0.0003	-500	1.10288	-312
	$J \pm (DP_1)$	1.10052 ±0.0003	-548	1.10370	-230
3 (0.8820±0.0079)	MOC	0.88593 ±0.0003	393	0.88609	409
	CP	0.88554 ±0.0003	354	0.88615	415
	$J \pm (DP_1)$	0.87523 ±0.0003	-677	0.87225	-975
4 (0.8360±0.0091)	MOC	0.84001 ±0.0003	401	0.84189	589
	CP	0.84123 ±0.0003	523	0.84192	592
	$J \pm (DP_1)$	0.82672 ±0.0003	-928	0.81301	-2299
5 (0.8140±0.0103)	MOC	0.79637 ±0.0003	-1763	0.81907	507
	CP	0.79600 ±0.0003	-1800	0.81909	509
	$J \pm (DP_1)$	0.79635 ±0.0003	-1765	0.80842	-558

Table II. LEU-COMP-THERM-041

Keeping in mind that experimental errors are quite large for this experience, numerical results show great concordance between Monte Carlo and S_N solutions. However, group constants obtained by a $J \pm (DP_1)$ in some cases lead to numerical oscillations for both S_N and Monte Carlo methods. A MOC or CP method is hence required in these 2D cases.

4. CONCLUSION

Combination of the lattice code DRAGON with its different subgroup based self-shielding models and the Monte Carlo code MORET has been successfully tested on more than 300 critical experiments coming from the ICSBEP. Results reveal consistency between self-shielding operators used with recently developed energy grids such as SHEM extented to 295 and 361 groups. The processing of DRAGLIB formated cross sections has been adapted to criticality-safety requirements, typically by adding missing isotopes and adjusting NJOY99 options. On another aspect, a modification of the lattice scheme is currently under development, leading to the use of a simplified Monte Carlo algorithm for the lattice calculation, i.e., the generation of multigroup constants.

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