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Technical note

Application of Tone's and embedded self-shielding methods to pressurized water reactor assemblies

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ABSTRACT

The Tone's and embedded self shielding methods are based on a heterogeneous-homogeneous equivalence principle. They both provide a formula for an *equivalent dilution parameter* that can be used to interpolate pretabulated effective cross sections for the infinite homogeneous medium. These two methods have been traditionally applied to fast reactor analysis with fine or ultrafine group energy mesh. We are investigating the accuracy of these two methods for the generation of self-shielded cross sections for typical pressurized water reactor assemblies.

1. Introduction

The purpose of the resonance self-shielding calculations in a lattice code is to produce averaged microscopic cross sections over coarse energy groups to be used later in a solution of the Boltzmann equation (Hébert, 2016). These calculations are based on different approximations:

1. A first class of resonant self-shielding models relies on the subgroup (or multiband) approach in which the detailed energy-dependent cross-section behaviour in each coarse energy group is replaced by its probability density representation (Levitt, 1972; Nikolaev, 1976). An accurate discretization of each probability density is then obtained, leading to quadrature sets called probability tables. These probability tables are subsequently used within the flux solution algorithm of the subgroup method. The subgroup projection method (SPM) is a recent implementation of the subgroup method available in the DRAGON5 lattice code (Hébert, 2009, 2016). Such method is considered the state-of-the-art for the generation of self-shielded cross sections for pressurized water reactor (PWR) assemblies.
2. Another class of methods are based on an heterogeneous-homogeneous equivalence principle. In this case, an *equivalent dilution parameter* $\sigma_{e,g}$ is computed for each resonant isotope, in each resonant region and each resonant energy group g. This dilution parameter is used to interpolate pretabulated effective cross sections for the infinite homogeneous medium, previously obtained with the *flux calculator* of the `GROUPR` module in code NJOY (MacFarlane and Kahler, 2010). This class of models originates from WIMS (Askew et al., 1966) and is still used in many legacy codes in some advanced form. Helpful extensions have been proposed by Stamm'ler(code PHOENIX) by introducing rational expansions of the fuel-to-fuel collision probabilities (Stamm'ler et al., 1977; Stamm'ler and Abbate, 1983). Other recognized equivalence techniques are the *Livolant-Jeanpierre* self-shielding method of the APOLLO1 lattice code and the *Sanchez-Coste* self-shielding method of the APOLLO2 lattice code, both of which are based on Lebesque integration (Livolant and Jeanpierre, 1974; Coste-Delclaux, 2006). In the seventies, the Tone's method was applied to fast reactor analysis with fine or ultrafine group energy mesh (Tone, 1975). Later, a similar technique known as the *embedded self-shielding method* (ESSM) was proposed (Hong and Kim, 2011; Williams and Kim, 2012). The ESSM allows self-shielded cross sections to be generated directly in the transport geometry without requiring external computation of Dancoff factors.

From a programming and implementation point of view, Tone's and embedded self-shielding methods are very close. Their applications on a simple pincell without submeshing of the fuel pin lead to the same numerical result. Both approaches can be implemented in a lattice code with little programming effort, as no probability tables or Dancoff factors need to be computed. Also, these techniques are CPU efficient and numerically stable, properties

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that are appreciated for computing doppler reactivity coefficients. Recently, the Tone's method was proposed by Mao and Zmijarevic for the conception of computational schemes for fast breeder reactor (FBR) lattice analyses, as an alternative to the subgroup approach that was previously used (Mao and Zmijarevic, 2017). Here, we should mention that the approach used by Mao and Zmijarevic is not based on an equivalence with pre-tabulated values obtained with the flux calculator in code NJOY. Instead, they recompute the effective cross sections at the correct dilution using a Bondarenko flux definition with a Lebesgue integration based on CALENDF probability tables.

They are some concerns about the applicability of Tone's and embedded self-shielding methods for the analysis of PWR assemblies. The ESSM is proposed for performing resonance self-shielding calculations in the POLARIS lattice code, a component of the SCALE system (Jessee et al., 2014). There is an important distinction between FBR and PWR assemblies. Distributed self-shielding effects are significant for PWR, mainly for ^{238}U isotope which is responsible for ^{239}Pu production. As proposed by Santamarina, PWR fuel pins are divided in four volumes: 50%, 30%, 15% and 5% and Uranium–Gadolinium (U-Gd) pins are divided in six volumes: 20%, 20%, 20%, 20%, 15% and 5%. This submeshing of the fuel pins, specific for PWR assembly calculations, is the main source of concern with the ESSM and Tone's method. Submeshing of the fuel is also the cause of the slight discrepancy between the numerical results obtained with these two approaches. This paper is an investigation of these discrepancies and a proposition for an improvement to the Tone's method that would help reduce the errors related to distributed effects.

The validation process is based on two different codes: DRAGON5 as a lattice code running the optimized scheme and SERPENT2 (Leppänen, 2007) as a burnup 0 stochastic reference. All SERPENT2 runs were performed with 4000 cycles of 4000 source neutrons each. Two kinds of validation is done: a microscopic study with a comparison of the absorption (capture + fission) rates split in two groups (below 0.625 *eV* as a thermal group and over 0.625 eV as a fast group) and the relative accuracy on the fission maps are compared. In addition, the effective multiplication factor k_{eff} is compared as a macroscopic system characteristic.

2. Theory

A few assumptions are made for the heavy slowing-down operator $\mathcal{R}^*\{\varphi(\boldsymbol{r},u)\}$ at energies where the resonance self-shielding model is applied. We assume that scattering by the absorber is elastic and isotropic in the centre of mass, and that the target nucleus is effectively at rest in the laboratory system. However, the scattering source at lethargy u' will reflect the true material temperature since elastic scattering cross sections are Doppler broadened. This representation is written

$$\frac{1}{N^*}\,\mathcal{R}^*\{\varphi(\boldsymbol{r},u)\} = \frac{1}{1-\alpha}\int_{u-\epsilon}^{u} du'\,\mathrm{e}^{u'-u}\,\sigma_{\mathrm{s}}^*(\boldsymbol{r},u')\,\varphi(\boldsymbol{r},u') \tag{1}$$

where N^* is the number density of the resonant isotope and $\sigma_{\mathrm{s}}^*(u)$ is the microscopic elastic scattering cross section of the resonant isotope.

The simplified transport Eqs. (4)–(73). in Section 4.2.5 of Hébert (2016) can be used to describe a heterogeneous case with a unique resonant isotope. Here, we consider its solution over a coarse group g where the non-resonant cross sections are assumed to be constant in lethargy. We write

$$\begin{aligned}&\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\varphi(\boldsymbol{r},u,\boldsymbol{\Omega}) + \Sigma(\boldsymbol{r},u)\,\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})\\ &\quad= \frac{1}{4\pi}\left[\Sigma^+(\boldsymbol{r}) + \mathcal{R}^*\{\varphi(\boldsymbol{r},u)\}\right]\end{aligned} \tag{2}$$

where $\Sigma(\boldsymbol{r},u)$ is the macroscopic total cross section and $\Sigma^+(\boldsymbol{r})$ is the macroscopic total cross section of the non-resonant isotopes at position $\boldsymbol{r}$. The *fine structure function* $\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})$ is a generalization to the heterogeneous case for the solution of the *flux calculator* in code NJOY.

A class of self-shielding methods are based on an equivalence over the coarse group g between the solution of the heterogeneous Eq. (2 and a solution the NJOY *flux calculator* for an infinite homogeneous medium at dilution $\sigma_{\mathrm{e},g}$, written as

$$\left[\sigma_{\mathrm{e},g} + \sigma^*(u)\right]\varphi(u) = \sigma_{\mathrm{e},g} + \frac{1}{N^*}\,\mathcal{R}^*\{\varphi(u)\} \tag{3}$$

where $\sigma^*(u)$ is the microscopic total cross section of the resonant isotope and where

$$\sigma_{\mathrm{e},g} = \frac{\Sigma^+}{N^*} \tag{4}$$

is the dilution of the resonant isotope in the infinite homogeneous medium.

Both Tone's and embedded self-shielding methods provide a simple formula to compute $\sigma_{\mathrm{e},g}$ for a heterogeneous medium in fundamental mode condition, i.e., in cases where the boundary conditions are conservative. These two methods are simpler than alternative approaches because they do not require the application of Lebesgue integration techniques similar to those used with the subgroup method, with the Livolant-Jeanpierre method in APOLLO1 or with the Sanchez-Coste method in APOLLO2. Moreover, they do not require the evaluation of Dancoff factors similar to those used in the WIMD-D family of codes. However, fine or ultrafine group energy mesh must be used to maintain self-shielding accuracy, particularly over main resonances. This characteristic may be considered as a drawback and require extended validation for specific energy meshes. In this study, we are proposing to use the SHEM295 mesh, which features 170 resonant energy groups between 4.6325 and 1.2277×10^5 eV (Hébert, 2009). The legacy SHEM281 mesh cannot be used because the energy groups in the resolved energy domain are too coarse (Hfaiedh, 2006). The SHEM281 mesh has only 57 resonant energy groups between 22.5 and 1.2277×10^5 eV which is insufficient to apply the Tone's and embedded self-shielding methods.

2.1. The embedded self-shielding method

All reported applications of the ESSM are based on the *intermediate resonance* (IM) representation of the heavy slowing-down operator $\mathcal{R}^*\{\varphi(\boldsymbol{r},u)\}$. This representation consists in assuming that the resonances of the resonant isotope are intermediate and that the corresponding heavy slowing-down operator can be represented by a linear combination of a *narrow resonance* (NR) and a *wide resonance* (WR) model (Goldstein and Cohen, 1962). We write

$$\frac{1}{N^*}\,\mathcal{R}^*\{\varphi(u)\} = \lambda_g\,\sigma_{\mathrm{p}}^* + (1-\lambda_g)\,\sigma_{\mathrm{s}}^*(u)\,\varphi(u) \quad \text{if} \quad u_{g-1} \leqslant u < u_g \tag{5}$$

where λ_g is the Goldstein-Cohen parameter, adjusted between 0 and 1, corresponding to WR and NR approximations, respectively.

We are proposing to replace this representation with the *statistical* (ST) heavy slowing-down model, based on the assumption that the resonances of the heavy isotope are narrow, numerous and statistically distributed in group g. This model is more accurate than the NR model where the resonances are assumed to be isolated, which is not the case at high energies.

We propose to represent the heavy slowing-down operator as the average over group g of the scattering reaction rate:

$$\frac{1}{N^*}\,\mathcal{R}^*\{\varphi(\boldsymbol{r},u)\} = \langle\sigma_{\mathrm{s}}^*(\boldsymbol{r})\,\varphi(\boldsymbol{r})\rangle_g \quad \text{if} \quad u_{g-1} \leqslant u < u_g. \tag{6}$$