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# CONSIDERING THE UP-SCATTERING IN RESONANCE INTERFERENCE TREATMENT IN APOLLO3®

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## ABSTRACT

The use of the exact elastic scattering in resonance domain introduces the neutron up-scattering which must be taken into account in the deterministic transport code. The existing resonance interference treatment method in APOLLO3® is not able to take into account the resonance up-scattering phenomenon, since this method employs the asymptotic scattering kernel in the calculation of the infinite homogeneous medium reaction rates of mixture. It is known that the use of the asymptotic kernel instead of the realistic free-gas model has non-negligible impact on the calculated results. In order to consider both the resonance interference phenomenon and the resonant up-scattering, the resonance interference factor method was implemented in APOLLO3®. The numerical results showed that this method gived good results in both k-eff values and reaction rates.

An improved method was also proposed for the solution of the mixture heterogeneous equation by the fine-structure self-shielding method. Compared to the existing method, it requires less storage memory and less solution time, but it gives the same numerical results as those of the existing method.

*Key Words*: resonance interference, up-scattering, resonance interference factor, resonance self-shielding, fine-structure method, APOLLO3®

## 1 INTRODUCTION

The fine-structure (FS) method is a self-shielding method based on equivalence theory [1–4]. It comprises two steps, both are based on the reaction rate preserving principle. The first one, called *heterogeneous-homogeneous equivalence*, is the application of the FS approximation in which the reaction rates of each region of a heterogeneous problem are calculated in an equivalent infinite homogeneous medium (IHM). Each IHM is characterized by an effective value of cross sections that preserves the reaction rates. The equivalent cross section is searched iteratively, where both heterogeneous and homogeneous problems are calculated using the identical scattering model and the identical numerical quadrature.

Such obtained equivalent cross section is used to calculate the final reaction rate in IHM by interpolation in the pretabulated IHM reaction rate tables, which are *problem independent* and are function of background cross section and of temperature. This final rate is considered to be the

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solution of heterogeneous problem for the self-shielding region. Finally, *continuous-to-multigroup equivalence* is performed in order to determine the multigroup cross sections.

In case of treating a mixture of resonant isotopes, the resonant isotopes in the mixture will be treated one-by-one: when one isotope is being treated, the other isotopes are considered as *background* isotopes, using its infinite dilution cross sections or its self-shielded cross sections if it has already been treated. This is the iterative method (Iter) in APOLLO2 [5] and APOLLO3® [6]. In this way, we can treat each isotope independently, using the *problem independent* preprocessed multigroup library. But the drawback of the Iter method is that it does not account for the mutual resonance shielding from the other resonant isotopes in the mixture. Examples were given to show that this approximate treatment can introduce significant errors in the self-shielding calculation of a mixture of resonant isotopes [3].

In order to remedy this problem, M. Coste [3, 7, 8] has implemented a mixture treatment in APOLLO2 which treats simultaneously all resonant isotopes in a mixture. Since isotopic proportions are not known before the calculation is set, this method computes on-the-fly the quadrature formulas for the mixture as a whole. Once the quadrature formulas are obtained, the heterogeneous-homogeneous equivalence is carried out to calculate the equivalent cross section for each resonant isotope in the mixture. A fine-mesh multigroup IHM calculation is effectuated on-the-fly for the mixture being treated in order to obtain the reference IHM reaction rates. This fine-mesh IHM calculation is carried out using the TR (Toute Résonance) slowing-down model and using the fine-mesh quadrature formulas. It is thus named TRF. When the energy mesh is refined enough, the IHM rates given by the TRF method were considered to be equivalent to those calculated by the NJOY nuclear data processing system without making approximation on the slowing-down model. This method is hereinafter called the Coste method.

The Coste method has diminished the error caused by mutual resonance shielding and the reaction rates agree well to those of the Monte Carlo reference calculation [3]. But it has several drawbacks. This method is relying on the on-the-fly tabulation of the IHM reaction rates of the mixture. In this fine-mesh IHM calculation, the fine-mesh temperature-dependent transfer cross-sections are not available because they are voluminous. Therefore the asymptotic transfer probabilities are employed instead of the exact transfer probabilities, that is, the temperature-dependence of the transfer cross-sections has been ignored. In our recent work of the resonant up-scattering treatment with the FS method in APOLLO3® [4], the Coste method can not be applied directly. The reason is that in case of the resonant up-scattering phenomenon introduced by the heavy isotopes, the transfer cross-sections are indeed temperature-dependent. The use of the asymptotic transfer kernel instead of the realistic free-gas model may have an impact far from negligible.

In order to account for both the resonance interference and the resonant up-scattering in APOLLO3®, we consider the Resonance Interference Factor (RIF) method introduced by M. L. Williams [9]. The RIF is the ratio between the self-shielded cross sections with and without the treatment of mutual resonance shielding. The resonant isotope is first self-shielded with the resonance interference neglected, and then the self-shielded cross-sections are corrected by applying the RIF.

A similar method was tested in the first version of the APOLLO2 by R. Sanchez and J. Mondot [2], which differed from Williams' method in that the RIF was defined as the ratio between the reaction rates with and without the consideration of resonance interference. The numerical results [2] showed that applying the RIF method to the FS self-shielding method efficiently reduced the error introduced by the mutual resonance shielding effects. Since the Sanchez & Mondot method was not retained in APOLLO2, and the quadrature formula needed by the implementation of the Wide-Resonance (WR) slowing-down model is not available in APOLLO3®, we decided to carry out the heterogeneous-homogeneous equivalence by the MD (Méthode Directe ) method of the Coste method. The IHM reaction rate tabulation was replaced by using the problem-independent preprocessed IHM reaction rate tables for single isotope, and applying the RIF to obtain the corrected reaction rates. The RIF is approximately calculated by applying the Statistical (ST) scattering model to the large-mesh IHM solution. This allows the consideration of mutual resonance shielding together with the consideration of the resonant up-scattering phenomenon.

Another improvement in the resonance interference treatment in APOLLO3® is the improvement in the MD method for solving the heterogeneous equation. In the old formalism, a coefficient matrix of dimensions $(N_\alpha, N_\alpha)$ per self-shielded resonant isotope has to be kept and a matrix of dimensions $(N_x \times N_\alpha, N_x \times N_\alpha)$ has to be inverted, where $N_x$ is the number of the resonant isotopes being treated simultaneously in mixture, and $N_\alpha$ is the number of self-shielding regions in the heterogeneous problem. This becomes a problem when the number of the resonant isotopes increases. An improved formalism was implemented in APOLLO3®. In the new formalism, all the resonant isotopes are treated as a whole, that is, as one single isotope. Only one coefficient matrix of dimensions $(N_\alpha, N_\alpha)$ is needed to be kept. The matrix to be inverted is also of dimensions $(N_\alpha, N_\alpha)$. This method is called the improved MD method (IMD). The numerical results showed that the IMD method gives the same results as those of the MD method.

In Section 2, we present the improvements in the resonance interference treatment by the FS self-shielding method in APOLLO3®. First, the IMD method is presented for the solution of the heterogeneous equation. Then the RIF method, which allows the resonance interference treatment when taking into account the resonant up-scattering, is described. In Section 3, the numerical results are given for the qualification of the new methods by two pin cell calculations, an UOX and a MOX cell calculations. First, three mixture treatments, the Iter, IMD+TRF and IMD+RIF methods, are compared to TRIPOLI-4® [10] calculations without considering the resonant up-scattering. Then the calculations with the consideration of the resonant up-scattering are carried out by the Iter and IMD+RIF methods. The results are compared to the TRIPOLI-4® [10] calculations with consideration of the resonant up-scattering.

## 2 IMPROVEMENTS IN RESONANCE INTERFERENCE TREATMENT

The FS method comprises of the following steps: the first step is the solution of the heterogeneous problem in order to obtain the heterogeneous reaction rates; the second step is to carry out the heterogeneous-homogeneous equivalence to obtain the equivalent cross-section for each self-shielding region; the third step is to interpolate with the equivalent cross-sections in the pre-tabulated IHM reaction rate tables, and to get the final reaction rates for each self-shielding region;

finally the continuous-to-multigroup equivalence is performed in order to determine the multigroup cross-sections.

In the following, only the new features in the resonance interference treatment will be presented. They concern the improved solution in the heterogeneous problem when considering the mutual resonance shielding, and the on-the-fly IHM reaction rate tabulation for a mixture of resonant isotopes. For the other features, such as the heterogeneous-homogeneous equivalence and the continuous-to-multigroup equivalence, the reader can refer to the previous work [3, 4, 11] for detailed description.

### 2.1 Heterogeneous Equation

For the heterogeneous problem, the collision probability equation is written as

$$\Sigma_i V_i \Phi_i = \sum_j P_{ij} V_j (R_{0j} \Phi_j + S_{1j}), \tag{1}$$

where $i, j$ are region indexes. $R_0$ is the resonant scattering operator, $S_1$ is the source term excluding the resonant contribution, $P_{ij}$ is the probability for a neutron born in region $j$ to have its first collision in region $i$, $\Phi$ is the scalar flux. $V$ is the region volume. $\Sigma$ is the total cross-section.

The self-shielding region (SSR) is introduced, which represents a set of flux calculation regions having, under the flat-flux assumption, an identical flux value,

$$\Phi_i = \Phi_\alpha, \quad \text{if} \quad i \in \alpha,$$

with $\alpha$ being the SSR index.

#### 2.1.1 The MD method

In the following, we first present the MD method for the solution of the heterogeneous equation. In the MD method, the following equation is obtained for a mixture of $N_x$ resonant isotopes:

$$\boldsymbol{\Phi}(u) = C(u) \boldsymbol{r}_0 \boldsymbol{\Phi}(u) + \boldsymbol{S}(u). \tag{2}$$

$\boldsymbol{\Phi}(u)$ is the flux; $C(u) = (C_1(u), C_2(u), \cdots, C_{N_x}(u))$ with $C_x(u)$ being the collision coefficient matrix for the $x$'th isotope, the elements of which are defined as $C_{x,\alpha\beta} = \dfrac{\sum_{i\in\alpha}\sum_{j\in\beta} P_{ij} V_j N_{0xj}}{\sum_{i\in\alpha}(\sum_y N_{0yi}\sigma_{0yi} + \Sigma_{1i}) V_i}$; $\boldsymbol{r}_0\boldsymbol{\Phi}(u)$ is the resonant scattering source, a vector of dimensions $(N_x \times N_\alpha)$; $\boldsymbol{S}(u)$ is the external source, with its elements defined as $S_\alpha = \dfrac{\sum_{i\in\alpha}\sum_j P_{ij}(u)\Sigma_{s1,j} V_j}{\sum_{i\in\alpha}(\sum_y N_{0yi}\sigma_{0yi} + \Sigma_{1i}) V_i}$. We observe that in Eq. (2), $C(u)$ is a matrix of dimensions $(N_\alpha, N_x \times N_\alpha)$.

The flat-source assumption is applied to the scattering source term. That is,

$$\boldsymbol{r}_0\boldsymbol{\Phi}(u) \approx (\boldsymbol{r}_0\boldsymbol{\Phi})^g = \frac{1}{\Delta u^g} \int_g \boldsymbol{r}_0\boldsymbol{\Phi}(u) du. \tag{3}$$

After that, the "Toutes Resonances" (TR) model [3] is employed to compute approximately the source term:

$$(\boldsymbol{r}_0\boldsymbol{\Phi})^g \approx \boldsymbol{r}_0\boldsymbol{\Phi}^{TR,g} = \left(\boldsymbol{r}_{01}\boldsymbol{\Phi}^{TR,g,T}, \boldsymbol{r}_{02}\boldsymbol{\Phi}^{TR,g,T}, \cdots, \boldsymbol{r}_{0N_x}\boldsymbol{\Phi}^{TR,g,T}\right)^T, \tag{4}$$

where

$$\boldsymbol{r}_{0x}\boldsymbol{\Phi}^{TR,g} = \sum_{g'} P_x^{g'\to g}\boldsymbol{\tau}_{s0x}^{TR,g'}, \tag{5}$$

and

$$\boldsymbol{\tau}_{s0x}^{TR,g} = \frac{1}{\Delta u^g}\int_g \sigma_{s0x}(u)\boldsymbol{\Phi}^{TR}(u)du. \tag{6}$$

$P_x^{g'\to g}$ is a diagonal matrix in respect to $g'$, with elements $p_x^{g'\to g}$, the probabilities for a neutron to scatter from group $g'$ to group $g$ after its collision with a nuclide of type $x$. $\sigma_{s0x}(u)$ is a diagonal matrix, with elements $\sigma_{s0x\alpha}(u)$. With these definitions, Eq. (4) becomes

$$\boldsymbol{r}_0\boldsymbol{\Phi}^{TR,g} = \sum_{g'} P^{g'\to g}\boldsymbol{\tau}_{s0}^{TR,g'}, \tag{7}$$

where $P^{g'\to g}$ is a block-diagonal matrix, with $P_x^{g'\to g}$ as its diagonal block. The scattering rate is

$$\boldsymbol{\tau}_{s0}^{TR,g} = \frac{1}{\Delta u^g}\int_g \sigma_{s0}(u)\boldsymbol{\Phi}^{TR}(u)du, \tag{8}$$

with the matrix of dimensions $(N_x \times N_\alpha, N_\alpha)$

$$\sigma_{s0}(u) = \left(\sigma_{s01}(u), \sigma_{s02}(u), \cdots, \sigma_{s0X}(u)\right)^T. \tag{9}$$

Inserting Eqs. (2) (7) into Eq. (8), we finally obtain

$$\begin{aligned}\boldsymbol{\tau}_{s0}^{TR,g} = &\left[1 - \frac{1}{\Delta u^g}\int_g \sigma_{s0}(u)C(u)P^{g\to g}du\right]^{-1} \\ &\times\left[\frac{1}{\Delta u^g}\int_g \sigma_{s0}(u)C(u)\sum_{g'\neq g} P^{g'\to g}\boldsymbol{\tau}_{s0}^{TR,g'}du + \frac{1}{\Delta u^g}\int_g \sigma_{s0}(u)\boldsymbol{S}(u)du\right].\end{aligned} \tag{10}$$

Once the scattering rates $\boldsymbol{\tau}_{s0}^{TR,g}$ are solved, we compute the scattering sources and the flux respectively by Eq. (7) and Eq. (2). The other reaction rates such as absorption can be calculated similarly as the scattering rates, see Eq. (8).

We note that the solution of Eq. (10) consists of inverting a matrix of dimensions $(N_x \times N_\alpha, N_x \times N_\alpha)$. It means that the more resonant isotopes being treated in the mixture, the bigger the coefficient matrix, the more memory is needed to keep it and the more CPU time is needed to invert it.

### 2.1.2 The improved MD method

From the upper description of the MD method, we obtain a system of equations of dimensions dependent on the number of resonant isotopes being treated. This makes the MD method less efficient compared to the traditional iterative (Iter) method, where the resonant isotopes are treated one-by-one and the linear system is always of dimensions $(N_\alpha, N_\alpha)$. In the following, we deduce a new system of equations more compact than that of the MD method.

We rewrite Eq. (2) in the following form

$$\boldsymbol{\Phi}(u) = C(u)\boldsymbol{r}_0\boldsymbol{\Phi}(u) + \boldsymbol{S}(u). \tag{11}$$

$\boldsymbol{\Phi}(u)$ and $\boldsymbol{S}(u)$ are the same as those in Eq. (2). But the matrix $C(u)$ now takes into account all resonant isotopes in mixture, its elements are defined as $C_{\alpha\beta} = \dfrac{\sum_{i\in\alpha}\sum_{j\in\beta} P_{ij}V_jN_{0j}}{\sum_{i\in\alpha}(\sum_y N_{0yi}\sigma_{0yi} + \Sigma_{1i})V_i}$, where $N_{0j} = \sum_x N_{0xj}$. The dimensions of the matrix $C(u)$ are $(N_\alpha, N_\alpha)$. $\boldsymbol{r}_0\boldsymbol{\Phi}(u)$ is the resonant scattering source, a vector of dimension $N_\alpha$.

The constant-in-energy source assumption is applied to the scattering source term. We have,

$$\boldsymbol{r}_0\boldsymbol{\Phi}(u) \approx (\boldsymbol{r}_0\boldsymbol{\Phi})^g. \tag{12}$$

Following the application of the TR assumption, we obtain

$$(\boldsymbol{r}_0\boldsymbol{\Phi})^g \approx (\boldsymbol{r}_0\boldsymbol{\Phi})^{TR,g} = \sum_{g'}(\boldsymbol{r}_0\boldsymbol{\Phi})^{TR,g'\to g}, \tag{13}$$

where

$$(\boldsymbol{r}_0\boldsymbol{\Phi})^{TR,g'\to g} = \sum_x A_x P_x^{g'\to g}\boldsymbol{\tau}_{s0x}^{TR,g'}, \tag{14}$$

with $A_x$ a diagonal matrix with elements $a_{0x\alpha} = N_{0x\alpha}/N_{0\alpha}$. $P_x^{g'\to g}$ is also a diagonal matrix, with elements $p_x^{g'\to g}$, the probability for a neutron to scatter from group $g'$ to group $g$ after its collision with a nuclide of type $x$. The scattering rates are defined as the following

$$\boldsymbol{\tau}_{s0x}^{TR,g} = \frac{1}{\Delta u^g}\int_g \sigma_{s0x}(u)\boldsymbol{\Phi}^{TR}(u)du, \tag{15}$$

where $\sigma_{s0x}(u)$ is a diagonal matrix, having elements $\sigma_{s0x\alpha}(u)$.

Therefore, we have the following equation for the scattering sources in group $g$,

$$(\boldsymbol{r}_0\boldsymbol{\Phi})^{TR,g\to g} = \sum_x A_x P_x^{g\to g}\frac{1}{\Delta u^g}\int_g \sigma_{s0x}(u)\boldsymbol{\Phi}^{TR}(u)du. \tag{16}$$

Inserting Eqs. (11) (12) (13) (15) into Eq. (16), after some arrangement, we obtain

$$
\begin{aligned}
(\boldsymbol{r}_0\boldsymbol{\Phi})^{TR,g\to g} = & \left[ I - \sum_x A_x P_x^{g\to g} \frac{1}{\Delta u^g} \int_g \sigma_{s0x}(u) C(u) du \right]^{-1} \\
& \times \Big( \sum_x A_x P_x^{g\to g} \frac{1}{\Delta u^g} \int_g \sigma_{s0x}(u) C(u) du \sum_{g'\neq g} (\boldsymbol{r}_0\boldsymbol{\Phi})^{TR,g'\to g} \\
& + \sum_x A_x P_x^{g\to g} \frac{1}{\Delta u^g} \int_g \sigma_{s0x}(u) \boldsymbol{S}(u) du \Big)
\end{aligned}
\tag{17}
$$

Once the scattering source from group $g$ $(\boldsymbol{r}_0\boldsymbol{\Phi})^{TR,g\to g}$ are known, the total scattering sources and the flux are respectively calculated by Eq. (13) and Eq. (11). The other reaction rates, such as absorption rates, can be calculated similarly as the scattering rates in Eq. (15).

We remark that in Eq. (17), the matrix to be inverted is of dimensions $(N_\alpha, N_\alpha)$, which are invariant regardless the number of the resonant isotopes being treated in mixture. Our numerical tests showed that the IMD method obtained the same numerical results as those of the MD method. However, compared to the MD method, only one coefficient matrix of dimensions $(N_\alpha, N_\alpha)$ instead of $N_x$ matrices is needed to be calculated and kept. The dimensions of the system of equations to be inverted decrease from $(N_x \times N_\alpha, N_x \times N_\alpha)$ to $(N_\alpha, N_\alpha)$.

The IMD method is capable to consider the resonant up-scattering phenomenon. The resonant up-scattering treatment implemented in the IMD method is similar to that implemented in the MD method [4].

Since both the MD and the IMD methods give the same numerical results, in our numerical tests, only the results for the IMD method are given.

## 2.2 The IHM Reaction Rate Tabulation For a Mixture

The resonance interference treatment by the FS method needs the on-the-fly IHM reaction rate tabulation, since the composition of mixture is only known once the problem is defined.

### 2.2.1 Fine-mesh TR method

In APOLLO3®, the Fine-mesh TR (TRF) method [3, 7, 8] was first implemented. In the TRF method, the TR model is applied to a fine-mesh IHM calculation for the mixture being treated and the reaction rates for each resonant isotopes are computed. The quadrature formulas used in this calculation are the fine-mesh probability tables, which are also needed to be computed on-the-fly. The fine-mesh employed in this calculation has about 11500 groups.

In the TRF method, the asymptotic transfer probabilities are employed instead of the exact transfer probabilities. This use of asymptotic scattering kernel instead of the realistic free gas model

was justified until the recent discovery of the resonant up-scattering phenomenon [12] caused by the scattering resonances of the heavy isotopes, specially U238. In our recent work of the resonant up-scattering treatment with the FS method in APOLLO3® [4], the TRF method can not be applied directly. The use of the asymptotic transfer kernel instead of the realistic free-gas model may have a non negligible impact on the reaction rates being calculated.

### 2.2.2 RIF method

In order to lift this limitation in the resonant interference treatment in the FS method, we consider the Resonance Interference Factor (RIF) method introduced by M. L. Williams [9]. In the work of Williams, the RIF is the ratio between the self-shielded cross sections with and without the consideration of mutual resonance shielding. In a similar method proposed by R. Sanchez and J. Mondot [2], the RIF was defined as the ratio between the reaction rates instead of the self-shielded cross sections.

In our implementation in APOLLO3®, we follow the Sanchez & Mondot definition of RIF, and the RIF are applied to the reaction rates. Since the quadrature formulas needed by the Wide-Resonance (WR) slowing-down model for the moment are not available in APOLLO3®, the RIF are calculated by using the Statistic (ST) slowing-down model. The RIF are defined as

$$RIF_{\rho x\alpha} = \frac{\tau^{hete}_{\rho x\alpha,mix}(\sigma_{ex\alpha})}{\tau^{hete}_{\rho x\alpha,iso}(\tilde{\sigma}_{ex\alpha})} \approx \frac{\tau^{IHM,ST}_{\rho x,mix}(\sigma_{ex\alpha})}{\tau^{IHM,ST}_{\rho x,iso}(\tilde{\sigma}_{ex\alpha})}, \tag{18}$$

where $\sigma_{ex\alpha},\ x = 1, \cdots, N_x,\ \alpha = 1, \cdots, N_\alpha$ are the equivalent dilutions from the heterogeneous-homogeneous equivalence step. They are calculated for each self-shielding region in the heterogeneous problem. $\rho$ denotes the reaction type, such as absorption, scattering or production. $\tilde{\sigma}_{ex\alpha}$ are the equivalent dilutions when all other resonant isotopes are considered to be moderators and their total cross-sections are changed to their potential cross-sections [2]:

$$\tilde{\sigma}_{ex\alpha} = (\sigma_{ex\alpha} + \sum_{y \neq x} a_{0y}\sigma_{py})/a_{0x} - \sigma_{px}, \tag{19}$$

where $a_{0x} = N_{0x}/N_0$ is the isotopic proportion of isotope $x$ in the mixture.

Here we have made an assumption that the RIF are geometry independent and they can be calculated in an IHM situation. As our first test in APOLLO3®, the ST slowing-down assumption is employed in the IHM problem solution. In Appendix A the solution of the IHM problem by the ST model is given.

Once the RIF are known, we have

$$\tau^{hete}_{\rho x\alpha,mix}(\sigma_{ex\alpha}) = \tau^{hete}_{\rho x\alpha,iso}(\tilde{\sigma}_{ex\alpha}) \times RIF_{\rho x\alpha}. \tag{20}$$

The interpolation with the equivalent cross-section $\tilde{\sigma}_{ex\alpha}$ is first carried out in the IHM reaction rate tables for a single isotope from the multigroup library, then the RIF are applied to obtain the corrected reaction rates.

## 3 NUMERICAL RESULTS

In order to qualify the new developments in resonance interference treatment, the calculations of a typical PWR fuel cell are carried out. Two fuel compositions, UOX and MOX, are tested. Three different conditions at temperatures of 574K, 974K and 1174K are calculated. In Table I and Table II the geometry and composition data are given.

**Table I. Fuel cell geometry**

| Region | Material | Temperature (K) | Radius, Pitch (cm) |
|---|---|---|---|
| Fuel | UO2, MOX | 574, 974, 1174 | 0.4096 |
| Clad | ZrNAT | 600 | 0.474875 |
| Moderator | H2O | 574 | 1.26194 |

**Table II. Material composition**

| Material | Isotope | Concentration ($10^{24}$ atom / cm3 ) | Material | Isotope | Concentration ($10^{24}$ atom / cm3 ) |
|---|---|---|---|---|---|
| UO2 | O16 | 4.57e-2* | MOX | O16 | 4.594e-2 |
| | U234 | 7.38e-6 | | U235 | 5.4228e-5 |
| | U235 | 8.56e-4 | | U236 | 2.63e-9 |
| | U236 | 1.37e-6 | | U238 | 2.14e-2 |
| | U238 | 2.2e-2 | | Pu238 | 3.125e-5 |
| Clad | Zr | 3.8e-2 | | Pu239 | 8.84e-4 |
| Moderator | H2O | 2.21e-2 | | Pu240 | 3.874e-4 |
| | B10 | 5.13e-6 | | Pu241 | 1.39e-4 |
| | B11 | 2.065e-5 | | Pu242 | 9.22e-5 |
| | | | | Am241 | 1.85e-5 |

* Read as $4.57 \times 10^{-2}$

The numerical tests showed that the two methods for solving the mixture heterogeneous equation, the MD method and the IMD method, gave the same numerical results. Consequently, only the IMD method will be tested in the following calculations. In the following, three self-shielding methods are tested. They are the Iter, IMD+TRF and IMD+RIF methods. Since the same IMD method is utilized in the last two methods, for simplifying the notation, the IMD+TRF method is denoted by the TRF method, and the IMD+RIF method is denoted by the RIF method.

### 3.1 Asymptotic kernel (AK) calculations

In order to qualify the newly implemented RIF method against the Iter method and the TRF method in APOLLO3®, the calculations were carried out using the CEA2005 V5.1.2 SHEM

**Table III. K-eff values on the UOX cell using asymptotic kernel**

| Temp. (K) | TRIPOLI-4® $\pm\sigma$ (pcm) | APOLLO3® Iter | $\Delta\rho$ (pcm) | APOLLO3® TRF | $\Delta\rho$ (pcm) | APOLLO3® RIF | $\Delta\rho$ (pcm) |
|---|---|---|---|---|---|---|---|
| 574 | 1.28415±7 | 1.28437 | 14 | 1.28453 | 23 | 1.28477 | 38 |
| 974 | 1.26906±7 | 1.26912 | 4 | 1.26937 | 19 | 1.26954 | 30 |
| 1174 | 1.26271±7 | 1.26217 | -33 | 1.26254 | -10 | 1.26292 | 13 |

**Table IV. K-eff values on the MOX cell using asymptotic kernel**

| Temp. (K) | TRIPOLI-4® $\pm\sigma$ (pcm) | APOLLO3® Iter | $\Delta\rho$ (pcm) | APOLLO3® TRF | $\Delta\rho$ (pcm) | APOLLO3® RIF | $\Delta\rho$ (pcm) |
|---|---|---|---|---|---|---|---|
| 574 | 1.11212±6 | 1.11184 | -22 | 1.11329 | 90 | 1.11347 | 109 |
| 974 | 1.09602±6 | 1.09543 | -49 | 1.09722 | 99 | 1.09742 | 116 |
| 1174 | 1.08930±6 | 1.08794 | -115 | 1.08991 | 52 | 1.09021 | 76 |

281-group library [13], which is based on the JEFF-3.1.1 nuclear data evaluation [14]. These calculations do not account for the resonant up-scattering phenomenon of the heavy isotopes, the transfer cross-sections for the heavy isotopes are generated using the asymptotic kernel. Since there is no up-scattering of the heavy isotopes, the TRF IHM reaction rate tabulation with the asymptotic kernel can be carried out. Therefore, it is possible to compare the TRF and the RIF methods.

The APOLLO3® calculations are compared to the TRIPOLI-4® Monte Carlo calculations. In the TRIPOLI-4® calculations, the traditional *Sampling of the Velocity of the Target nucleus* (SVT) model [15] was used, the up-scattering phenomenon was ignored. The self-shielding calculations of APOLLO3® were carried out respectively by the Iter method, the IMD method plus the TRF method and the IMD method plus the RIF method. The TR scattering model was employed in the heterogeneous-homogeneous equivalence of three calculations. The multigroup flux calculation was carried out by the method of characteristics. The results are given in Tables III and IV. From the comparison of the k-eff values, we notice that in some cases the iterative treatment (Iter) gives the k-eff's closer to those of TRIPOLI-4® than the other two methods. The RIF method gives the results close to those of the TRF method, but the TRF method gives better results.

The Comparisons of the absorption rates are given in Figures 1 and 2, for the two most important resonant isotopes, U238 and Pu239, in the 1174K MOX cell calculation. We notice that the good results of the Iter method in k-eff come from the cancellation of the large discrepancies in reaction rates. This cancellation changes with the temperature, that is why the error in k-eff changes with temperature. The TRF method gives the absorption rates closest to those of the references. The RIF method gives rather good results close to those of the TRF method, even though it is much simpler in theory and implementation.

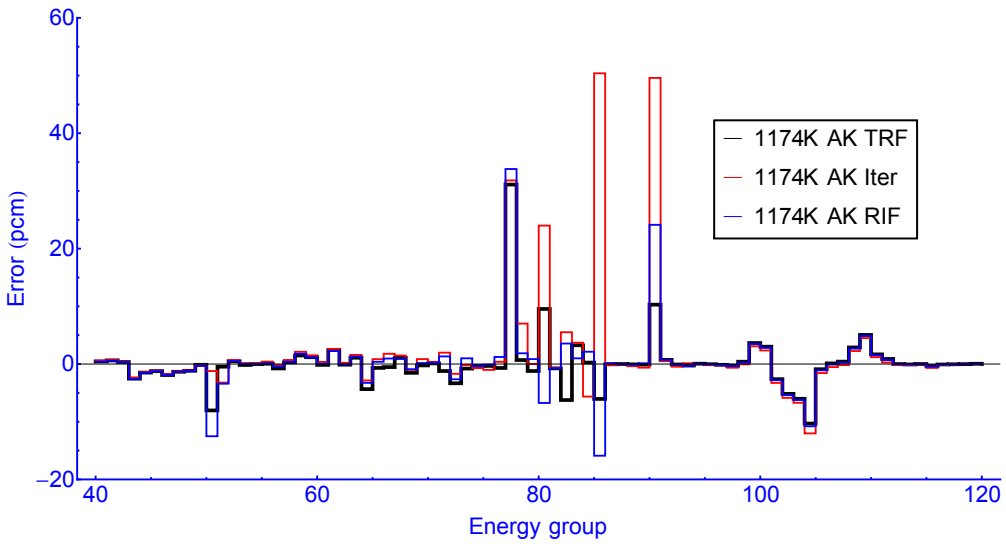



**Figure 1. Differences of APOLLO3® resonance interference treatments in U238 absorption rate errors in MOX cell.**

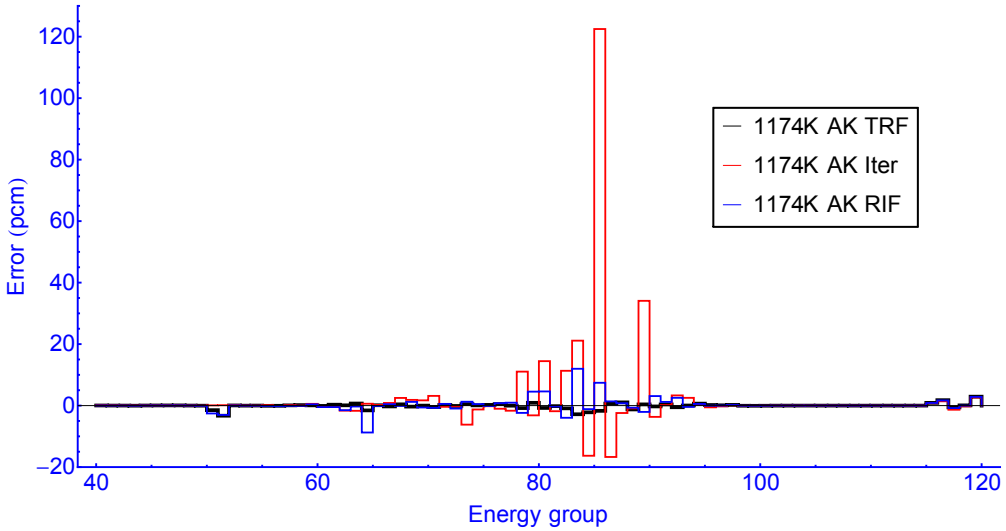



**Figure 2. Differences of APOLLO3® resonance interference treatments in Pu239 absorption rate errors in MOX cell.**

### 3.2 Up-scattering (UpSc) calculations

In the calculations considering the resonance up-scattering phenomenon, only the Iter and RIF methods can be applied. The calculations are carried out by employing the newly produced CEA2005 V5.1.2-UPS library. It is also based on the JEFF-3.1.1 nuclear data evaluation [14]. The transfer matrices for U238, Pu240 and Pu242 are produced using the newly developed free-gas

model [16], by the new library processing system GALILEE V0.3 [17, 18]. The up-scattering threshold is chosen to be 360 eV. For the free hydrogen as well as for the hydrogen and oxygen bound in water, the thermal cut-off is also modified to 360 eV. The energy mesh is SHEM 281 group [13].

The APOLLO3® calculations are compared to the TRIPOLI-4® Monte Carlo calculations. In the TRIPOLI-4® calculations, the up-scattering phenomenon was taken into account by the newly implemented *Doppler Broadening Rejection Correction* (DBRC) model [15, 19]. The self-shielding calculations of APOLLO3® were carried out respectively by the Iter method and the IMD+RIF method. The TR model was employed in the heterogeneous-homogeneous equivalence stage of the calculations. The multigroup flux calculation was carried out by the method of characteristics.

The comparison of the Iter and RIF methods is given for the UOX and MOX cell respectively in Tables V and VI. We remark that both Iter and RIF methods give k-eff's close to those of TRIPOLI-4®. In both UOX and MOX cell calculations, the error in k-eff increases with temperature for the Iter method; whereas the error in k-eff decreases with temperature for RIF method.

**Table V. K-eff values on the UOX cell with resonant up-scattering**

| Temp. (K) | TRIPOLI-4® $\pm\sigma$ (pcm) | APOLLO3® Iter | $\Delta\rho$ (pcm) | APOLLO3® RIF | $\Delta\rho$ (pcm) |
|---|---|---|---|---|---|
| 574 | 1.28246±7 | 1.28258 | 8 | 1.28301 | 34 |
| 974 | 1.26654±7 | 1.26631 | -15 | 1.26677 | 14 |
| 1174 | 1.25947±7 | 1.25890 | -36 | 1.25970 | 14 |

**Table VI. K-eff values on the MOX cell with resonant up-scattering**

| Temp. (K) | TRIPOLI-4® $\pm\sigma$ (pcm) | APOLLO3® Iter | $\Delta\rho$ (pcm) | APOLLO3® RIF | $\Delta\rho$ (pcm) |
|---|---|---|---|---|---|
| 574 | 1.10999±6 | 1.10931 | -55 | 1.11094 | 77 |
| 974 | 1.09307±6 | 1.09196 | -93 | 1.09394 | 73 |
| 1174 | 1.08573±6 | 1.08406 | -142 | 1.08633 | 51 |

The Comparisons of the absorption rates are given in Figures 3 and 4, for U238 and Pu239, in the 1174K MOX cell calculation with consideration of resonance up-scattering. We notice the similar behavior to that of the asymptotic kernel calculations. The good performance of the Iter method in k-eff's came from the cancellation of the large discrepancies. Since the cancellation changes with the temperature, that is why the error in k-eff changes greatly with temperature. The RIF method gives rather good agreement in reaction rates with those of the Monte Carlo reference.

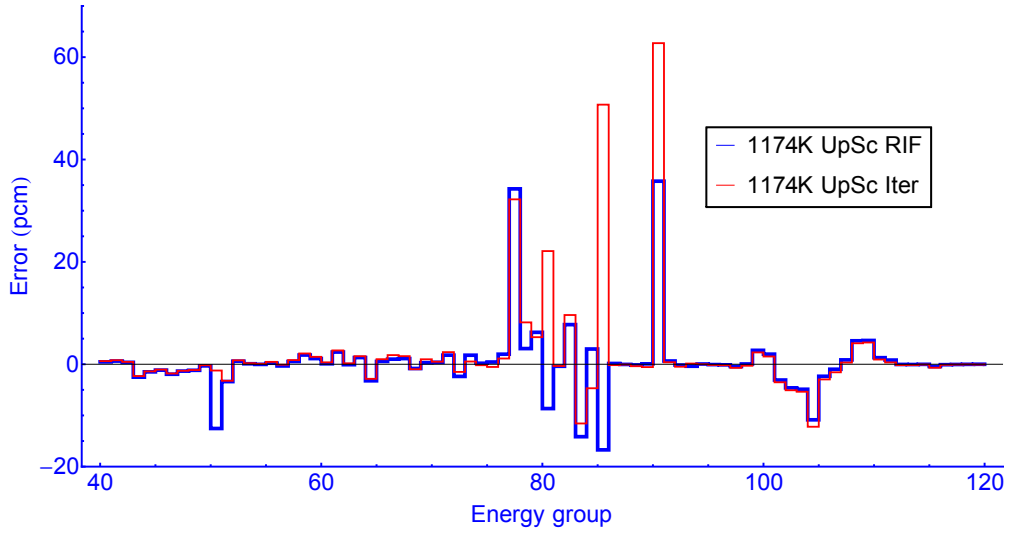



**Figure 3. Differences of APOLLO3® resonance interference treatments in U238 absorption rate errors in MOX cell.**

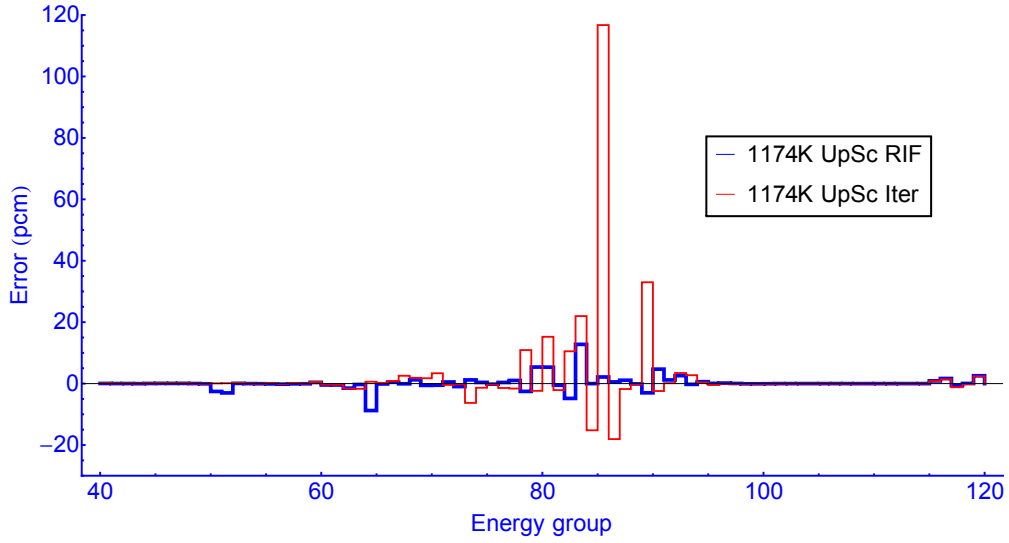



**Figure 4. Differences of APOLLO3® resonance interference treatments in Pu239 absorption rate errors in MOX cell.**

## 4 CONCLUSIONS

In this paper, the new resonance interference treatments in APOLLO3® have been presented. We first describe the improved MD method formalism for the solution of the heterogeneous equation in mixture treatment. The IMD and MD methods give the same numerical results, but the IMD

method allows the solution of the heterogeneous equation to use less memory and less CPU time compared to the MD method.

The RIF method combined with the IMD method makes it possible to treat simultaneously the resonance interference and the resonant up-scattering phenomenon. In the asymptotic kernel calculations, three methods, Iter, TRF and RIF, are compared. The numerical results showed that the Iter method gives good approximation in k-eff, but it is because of the cancellation of large discrepancies in reaction rates. The TRF and RIF methods remedy well these discrepancies. The TRF gives closer results to those of TRIPOLI-4®, but the RIF is simpler in implementation.

As the TRF method can not be applied to the up-scattering calculations, only the Iter and RIF methods are used in the up-scattering calculations. Their behaviors are similar to those in asymptotic kernel calculations. The RIF method is a simple and fast method which remedies quite well the resonance interference phenomenon in the fine-structure self-shielding calculation in APOLLO3®.

## 5 ACKNOWLEDGMENTS

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## APPENDIX A SOLUTION OF THE IHM PROBLEM BY THE STATISTICAL (ST) MODEL

We consider an infinite homogeneous medium filled with a mixture of $N_x$ resonant isotopes and moderator isotopes. The following equation is established

$$\left(\sum_x N_{0x}\sigma_{0x} + \Sigma_1\right)\Phi = \sum_x N_{0x} r_{0x}\Phi + \Sigma_{s1}\chi, \tag{21}$$

where $0$ and $1$ represent respectively resonant and moderator isotopes, $R\Phi = Nr\Phi$ is the scattering source. $\Sigma$ and $\Sigma_s$ are respectively the total and scattering cross-section. $\chi = \dfrac{R_1\Phi}{\Sigma_{s1}}$ is a global

slowly-varying *macroscopic flux*. It is assumed that $\Phi = \chi\phi$, where $\phi$ is a local fast-varying *fine-structure factor*. By applying the fine-structure assumption, $r_{0x}\Phi \approx \chi r_{0x}\phi$, we get

$$(\sigma_0(u) + \sigma_b)\phi(u) = \boldsymbol{a}^T \boldsymbol{r_0}\boldsymbol{\phi} + \gamma_b\sigma_b, \tag{22}$$

with $\sigma_0(u) = \boldsymbol{a}^T\boldsymbol{\sigma}_0(u)$, $\boldsymbol{a} = (a_{01}, \cdots, a_{0N_x})^T$, $\boldsymbol{\sigma}_0(u) = (\sigma_{01}(u), \cdots, \sigma_{0N_x}(u))^T$, and $a_{0x} = N_{0x}/N_0$, $N_0 = \sum_x N_{0x}$, $\gamma_b = \Sigma_{s1}/\Sigma_1$, $\sigma_b = \Sigma_1/N_0$. The scattering source is obtained by applying the ST model,

$$\boldsymbol{r_0}\boldsymbol{\phi} \approx \boldsymbol{r_0}\boldsymbol{\phi}^{ST,g} = \boldsymbol{\tau}_{s0}^{ST,g}, \tag{23}$$

where $\boldsymbol{\tau}_{s0}^{ST,g}$ is the scattering rate of group $g$, defined as

$$\boldsymbol{\tau}_{s0}^{ST,g} = \frac{1}{\Delta u^g}\int_g \boldsymbol{\sigma}_{s0}(u)\phi(u)du, \tag{24}$$

with $\boldsymbol{\sigma}_{s0}(u) = (\sigma_{s01}(u), \cdots, \sigma_{s0N_x}(u))^T$.

From Eqs. (22) (23) (24), we obtain the solution for the scattering source,

$$\boldsymbol{\tau}_{s0}^{ST,g} = \boldsymbol{I}_{s0}^g \frac{\gamma_b\sigma_b}{1 - \boldsymbol{a}^T\boldsymbol{I}_{s0}^g}, \tag{25}$$

with

$$\boldsymbol{I}_{s0}^g = \frac{1}{\Delta u^g}\int_g \frac{\boldsymbol{\sigma}_{s0}(u)}{\sigma_0(u) + \sigma_b}du. \tag{26}$$

The reaction rates for a reaction of type $\rho$ are calculated by

$$\boldsymbol{\tau}_{\rho0}^{ST,g} = \boldsymbol{I}_{\rho0}^g \frac{\gamma_b\sigma_b}{1 - \boldsymbol{a}^T\boldsymbol{I}_{s0}^g}, \tag{27}$$

with

$$\boldsymbol{I}_{\rho0}^g = \frac{1}{\Delta u^g}\int_g \frac{\boldsymbol{\sigma}_{\rho0}(u)}{\sigma_0(u) + \sigma_b}du. \tag{28}$$