

NEW RESONANT MIXTURE SELF-SHIELDING TREATMENT IN THE CODE APOLLO2

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Up to now, the self-shielding module of the multigroup transport code APOLLO2 [1] could treat one resonant isotope mixed with moderator isotopes. Consequently, the resonant mixture self-shielding treatment was an iterative one. Each resonant isotope of the mixture was treated separately, the other resonant isotopes of the mixture being then considered as moderator isotopes, that is to say non-resonant isotopes. This treatment could be iterated. This approximate method could lead to discrepancies (versus reference calculations) of several percents on the resonant absorption reaction rates.

The new method consists in treating the resonant mixture as a unique entity. New developments were carried out to take into account (with the Livolant-Jeanpierre approach) this global entity, to dynamically recalculate in the code APOLLO2 the self-shielding data of the treated mixture and then to perform separately the self-shielded cross-sections of each component of the mixture.

This new treatment allows us to reduce the local discrepancies on resonant absorption reaction rates versus reference calculations. However, as this new method suppresses compensations, some global results such as effective multiplication factor can be slightly deteriorated.

KEYWORDS: *Self-shielding formalism, resonant mixture, multigroup transport code, APOLLO2*

1 Introduction

APOLLO2 is a modular multigroup transport code developed at the Commissariat à l'Énergie Atomique at SACLAY. An early approximate model was proposed by R. SANCHEZ and J. MONDOT [2] in 1984 but was not kept in APOLLO2. Consequently, up to now, the self-shielding module could only treat one resonant isotope mixed with moderator isotopes. Consequently, the resonant mixture self-shielding treatment was an iterative one. Each resonant isotope of the mixture was treated separately, the other resonant isotopes of the mixture being then considered as moderator isotopes, that is to say non-resonant isotopes. This treatment could be iterated.

There are two different ways to perform a self-shielding calculation in the code APOLLO2. In industrial APOLLO2 versions, the self-shielding calculation uses the Livolant-Jeanpierre approach based on a double equivalence. In reference calculations performed with APOLLO2 working on a very fine energy mesh, or in the unresolved resonance range of a resonant iso-

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tope, the self-shielding calculation uses the sub-group approach. The new method for treating resonant mixtures has been implemented in the Livolant-Jeanpierre approach, but it could be implemented in a very similar way in the sub-group approach.

Let us come back to the Livolant-Jeanpierre approach. It is carried out by two steps: first a homogenization which gives for a given resonant isotope, the reaction rates in a heterogeneous geometry by interpolating "exactly" calculated homogeneous reactions rates versus an equivalent background cross-section, and then a multigroup equivalence which gives the self-shielded cross-sections of the treated isotope. We detail a little these two steps.

In the homogenization step, we compute for each resonant group and each self-shielding region the partial reaction rates of the treated resonant isotope (absorption, scattering and production). This is achieved by calculating first an approximate slowing-down flux given by a fine structure equation in which the slowing-down operator of the resonant isotope is modelled. Then, we look for an equivalent background cross-section characterizing an infinite homogeneous medium with the same absorption rate (evaluated with the same slowing-down model as in the heterogeneous calculation). We recall that we have at our disposal, in APOLLO2 libraries, quadrature formulas to calculate reaction rates in terms of a known flux and homogeneous partial reaction rate tabulations versus temperature and background cross-section. (These tabulations are calculated by the NJOY nuclear data processing system [3] with an "exact" slowing-down operator.) Consequently, by interpolating in the tabulations at the equivalent background cross-section value, we deduce the "exact" partial reaction rates in each resonant group and each self-shielding region. This step is the tricky one because it needs physical modelling.

In the multigroup equivalence step, we have to solve a non-linear system giving, for each resonant isotope, the multigroup cross-sections that preserve the partial reaction rates obtained at the homogenization step. This step is mainly a numerical one.

2 New resonant mixture treatment

In order to explain the new resonant mixture treatment, we will consider each step of the self-shielding calculation and we will detail the developments that we had to carry out.

2.1 Homogenization

There is a main difference between the treatment of one resonant isotope or the direct treatment of a resonant mixture. What we need in the flux calculation is not the mixture self-shielded cross-sections but the self-shielded cross-sections of each component of the mixture. Consequently, the homogenization step will have to provide, in each self-shielding region and each resonant group, the "exact" reaction rates of each resonant isotope of the mixture.

In order to achieve the homogenization step in the frame of a given resonant mixture, we have to solve the fine structure slowing-down equation written for the mixture in heterogeneous geometry and for that, we need a slowing-down model for the mixture. Once the approximate flux is known, we need quadrature formulas to calculate the mixture absorption reaction rate and to perform the equivalent background cross-section. Finally, we need, for each component of the mixture, homogeneous tabulations performed with an "exact" slowing-down operator. That will give the "exact" partial reaction rates for each isotope of the mixture.

We describe now the original work. We note with index m varying from 1 to M , the various isotopes of the resonant mixture.

In a homogeneous medium characterized by a background cross-section σ_b and an absorption power γ_b , the flux is given by the fine structure equation:

$$\left(\sum_{m=1}^M a_{0m} \sigma_{0m} + \sigma_b\right) \varphi = \sum_{m=1}^M a_{0m} r_{0m} \varphi + \gamma_b \sigma_b \quad (1),$$

where a_{0m} is the relative proportion of the isotope m in the resonant mixture, σ_{0m} its total microscopic cross-section and r_{0m} the microscopic slowing-down operator.

In heterogeneous geometry, the fine structure equation can be written in the following way:

$$\varphi_0 = C \mathcal{R}_0 \varphi_0 + S \quad (2),$$

where the matrix C , the source S and the slowing down operator are defined by :

$$C_{\alpha\beta} = \frac{\sum_{i \in \alpha} \sum_{j \in \beta} P_{ij} V_j N_{0j}}{\sum_{i \in \alpha} \left(\left(\sum_{\ell=1}^M N_{0\ell i} \sigma_{0\ell i} \right) + \Sigma_{li} \right) V_i}, S_{\alpha} = \frac{\sum_{i \in \alpha} \sum_j P_{ij} V_j \Sigma_{s1j}}{\sum_{i \in \alpha} \left(\left(\sum_{\ell=1}^M N_{0\ell i} \sigma_{0\ell i} \right) + \Sigma_{li} \right) V_i}, \mathcal{R}_{0\alpha} \varphi_{0\alpha} = \sum_{m=1}^M a_{0m\alpha} r_{0m\alpha} \varphi_{0\alpha} \quad (3).$$

Let α and β be two self-shielding regions. The notation is the following one: P_{ij} is the probability for a neutron born in region j to have its first collision in region i , V_j is the volume of region j , N_{0j} is the total resonant concentration in region j , Σ_{li} and Σ_{s1i} are respectively the total macroscopic cross-section and the scattering macroscopic cross-section of the moderator isotopes in region i . The relative proportion (resp. the microscopic resonant cross-section and the microscopic slowing-down operator) of isotope m in the resonant mixture present in region α is given by $a_{0m\alpha}$ (resp. $\sigma_{0m\alpha}$ and $r_{0m\alpha}$).

In that treatment we use for each resonant isotope the TR slowing-down model allowing us to model the slowing-down operator, whatever the resonance shape is. We recall that the TR model for a resonant slowing-down operator is given by:

$$r_{0m\alpha}^{\text{TR}} \varphi_{0\alpha}(u) = \sum_{g' \leq g} \text{prop}_m(g', g) \langle \sigma_{s0m\alpha} \varphi_{0\alpha} \rangle^{g'} \quad \text{for } u \in g,$$

$\langle \sigma_{s0m} \varphi_{0\alpha} \rangle^{g'}$ being the mean scattering reaction rate in region α and group g' and $\text{prop}_m(g', g)$ the mean probability, for isotope m , of scattering from group g' to group g .

2.1.1 Homogeneous reaction rate calculation with the TR model

We use the TR model in the homogeneous equation (1). We obtain:

$$\begin{cases} \left(\sum_{m=1}^M a_{0m} \sigma_{0m}(u) + \sigma_b\right) \varphi(u) \approx \sum_{m=1}^M a_{0m} r_{0m}^{\text{TR}} \varphi(u) + \gamma_b \sigma_b \\ r_{0m}^{\text{TR}} \varphi(u) = \sum_{g' \leq g} \text{prop}_m(g', g) \langle \sigma_{s0m} \varphi \rangle^{g'} \quad \text{when } u \in g \end{cases} \quad (4).$$

The mean scattering reaction rate is calculated by using the φ value given by equation (4):

$$\langle \sigma_{s0m} \varphi \rangle^g = \frac{1}{\Delta u^g} \left[\sum_{\ell=1}^M a_{0\ell} \sum_{g' \leq g} \text{prop}_{\ell}(g', g) \langle \sigma_{s0\ell} \varphi \rangle^{g'} + \gamma_b \sigma_b \right] \int_g \frac{\sigma_{s0m}(u')}{\sum_{\ell=1}^M a_{0\ell} \sigma_{0\ell}(u') + \sigma_b} du'.$$

We note:

$$K_m^g = \sum_{g' < g} \text{prop}_m(g', g) \langle \sigma_{s0m} \phi \rangle^{g'}, \quad I_m^g = \frac{1}{\Delta u^g} \int_g \frac{\sigma_{s0m}(u')}{\sum_{\ell=1}^M a_{0\ell} \sigma_{0\ell}(u') + \sigma_b} du'.$$

The scattering reaction rates on the various groups are calculated by increasing lethargy. Consequently, when we want to evaluate $\langle \sigma_{s0m} \phi \rangle^g$, all the reaction rates $\langle \sigma_{s0\ell} \phi \rangle^{g'}$ for $1 \leq \ell \leq M$ and $g' < g$ are already known. The quantities K_ℓ^g are then constants that we know. The I_m^g integral is performed by a quadrature formula suited to the treated mixture that will be explained in §2.3. We can write:

$$\langle \sigma_{s0m} \phi \rangle^g = \left(\sum_{\ell=1}^M a_{0\ell} K_\ell^g + \sum_{\ell=1}^M a_{0\ell} \text{prop}_\ell(g, g) \langle \sigma_{s0\ell} \phi \rangle^g + \gamma_b \sigma_b \right) I_m^g.$$

We have to solve a linear system that can be written as:

$$(1 - a_{0m} \text{prop}_m(g, g) I_m^g) \langle \sigma_{s0m} \phi \rangle^g - I_m^g \sum_{\substack{\ell=1 \\ \ell \neq m}}^M a_{0\ell} \text{prop}_\ell(g, g) \langle \sigma_{s0\ell} \phi \rangle^g = \left(\sum_{\ell=1}^M a_{0\ell} K_\ell^g + \gamma_b \sigma_b \right) I_m^g \quad (5).$$

We can note that the expression:

$$\langle \sigma_{s0m} \phi \rangle^g = \frac{\left(\sum_{\ell=1}^M a_{0\ell} K_\ell^g + \gamma_b \sigma_b \right) I_m^g}{1 - \sum_{\ell=1}^M a_{0\ell} \text{prop}_\ell(g, g) I_\ell^g} \quad (6),$$

is solution of the system (5). To simplify the expressions, we set:

$$\lambda^g = \sum_{\ell=1}^M a_{0\ell} K_\ell^g + \gamma_b \sigma_b, \quad \mu^g = 1 - \sum_{\ell=1}^M a_{0\ell} \text{prop}_\ell(g, g) I_\ell^g.$$

By putting expression (6) in system (5), we obtain:

$$(1 - a_{0m} \text{prop}_m(g, g) I_m^g) \frac{\lambda^g I_m^g}{\mu^g} - I_m^g \sum_{\substack{\ell=1 \\ \ell \neq m}}^M a_{0\ell} \text{prop}_\ell(g, g) \frac{\lambda^g I_\ell^g}{\mu^g} = \lambda^g I_m^g.$$

The approximate TR flux is then given, for each lethargy u in the group g , by:

$$\phi^{\text{TR}}(u) = \frac{\lambda^g}{\mu^g} \frac{1}{\sum_{m=1}^M a_{0m} \sigma_{0m}(u) + \sigma_b} \quad (7).$$

We define the microscopic absorption rate of the mixture in the group g by:

$$T_{a0}^{g, \text{TR}} = \int_g \left(\sum_{m=1}^M a_{0m} \sigma_{a0m}(u) \right) \phi^{\text{TR}}(u) du \quad (8).$$

This reaction rate will be performed by a specific quadrature formula explained in §2.3.

2.1.2 Heterogeneous reaction rate calculation with the TR model

We use the TR model, for each resonant isotope, in heterogeneous equation (2). We obtain:

$$\left\{ \begin{array}{l} \Phi_{0\alpha} = \sum_{m=1}^M \sum_{\beta} C_{\alpha\beta} a_{0m\beta} r_{0m\beta} \Phi_{0\beta} + S_{\alpha} \\ r_{0m\beta}^{\text{TR}} \Phi_{0\beta}(u) = \sum_{g' \leq g} \text{prop}_m(g', g) \langle \sigma_{s0m\beta} \Phi_{0\beta} \rangle^{g'} \quad \text{when } u \in g \end{array} \right. \quad (9).$$

To simplify the expressions, we set: $C_{m,\alpha\beta} = a_{0m\beta} C_{\alpha\beta}$.

We determine the mean scattering rates in each self-shielding region α and each group g :

$$\begin{aligned} \langle \sigma_{s0m\alpha} \Phi_{0\alpha} \rangle^g &= \frac{1}{\Delta u^g} \int_g \sigma_{s0m\alpha}(u') \left(\sum_{\ell=1}^M \sum_{\beta} C_{\ell,\alpha\beta}(u') \sum_{g' < g} \text{prop}_{\ell}(g', g) \langle \sigma_{s0\ell\beta} \Phi_{0\beta} \rangle^{g'} + S_{\alpha}(u') \right) du' \\ &+ \frac{1}{\Delta u^g} \int_g \sigma_{s0m\alpha}(u') \left(\sum_{\ell=1}^M \sum_{\beta} C_{\ell,\alpha\beta}(u') \text{prop}_{\ell}(g, g) \langle \sigma_{s0\ell\beta} \Phi_{0\beta} \rangle^g \right) du' \end{aligned}$$

Let NRC be the self-shielding region number and M the resonant isotope number. Let us set $Q = \text{NRC} * M$ and let us define, for each group g , the Q-order vector, D^g and the Q-order square matrix V^g by:

$$\begin{aligned} D_{(\alpha,m)}^g &= \frac{1}{\Delta u^g} \sum_{\ell=1}^M \sum_{\beta} \sum_{g' < g} \text{prop}_{\ell}(g', g) \langle \sigma_{s0\ell\beta} \Phi_{0\beta} \rangle^{g'} \int_g \sigma_{s0m,\alpha}(u') C_{\ell,\alpha\beta}(u') du' \\ &+ \frac{1}{\Delta u^g} \int_g \sigma_{s0m\alpha}(u') S_{\alpha}(u') du' \\ V_{(\alpha,m),(\beta,\ell)}^g &= \delta_{(\alpha,m),(\beta,\ell)} - \frac{1}{\Delta u^g} \text{prop}_{\ell}(g, g) \int_g \sigma_{s0m,\alpha}(u') C_{\ell,\alpha\beta}(u') du'. \end{aligned}$$

The Q-order vector, $\langle \sigma_{s0} \Phi_0 \rangle^g$, whose components are $\langle \sigma_{s0m\alpha} \Phi_{0\alpha} \rangle^g$ is then given by:

$$\langle \sigma_{s0} \Phi_0 \rangle^g = V^{g-1} D^g \quad (10).$$

The integrals present in vector D^g or matrix V^g are performed with specific quadrature formulas described in §2.3.

Once vector $\langle \sigma_{s0} \Phi_0 \rangle^g$ is known, the approximate flux obtained with model TR in self-shielding region α is given by expression (9). The mixture microscopic absorption rate in each self-shielding region α and each resonant group g will be defined by:

$$T_{a0\alpha}^{g,\text{TR}} = \int_g \left(\sum_{m=1}^M a_{0m\alpha} \sigma_{a0m\alpha}(u) \right) \Phi_{0\alpha}^{\text{TR}}(u) du \quad (11).$$

It will be computed with specific quadrature formulas described in §2.3.

2.1.3 Reaction rates to be preserved

First, we calculate, for each resonant group g and each self-shielding region α the equivalent background cross-section that preserves in an infinite homogeneous medium the resonant mixture absorption rate carried out with model TR. Then, for each resonant isotope, we need

to know “exact” homogeneous partial reaction rates calculated, without modelling the slowing-down operator, for the equivalent background cross-section.

Contrary to the treatment of one resonant isotope, for a given mixture, the “exact” solution of the fine structure equation for the equivalent background cross-section (1) cannot be carried out at the multigroup library step. This “exact” solution will be calculated dynamically in the code APOLLO2 by using for the resonant slowing down operators the TR model applied on the very fine energy mesh used in the libraries to describe the partial cross-sections of the various resonant isotopes (~10 000 groups). The integrals that appear when we calculate the flux or the partial reaction rates (absorption, scattering, production) will be directly obtained from the very fine multigroup discretization of the partial cross-sections. These data already exist in present multigroup libraries for absorption and scattering cross-sections. They will be added for production cross-sections.

2.2 Multigroup equivalence

This step is formally the same as for one isotope and did not need any new development. [1]

2.3 Quadrature formulas

By making the assumption that the resonant mixtures are the same in all the self-shielding regions, that is to say, same isotopes, same temperatures and same relative concentrations, the integrals that we have to carry out in this treatment are of the following forms:

$$\int_g \sigma_{s0m}(u) f\left(\sum_{\ell=1}^M a_{0\ell} \sigma_{0\ell}(u)\right) du \quad \text{and} \quad \int_g \sigma_{a0m}(u) f\left(\sum_{\ell=1}^M a_{0\ell} \sigma_{0\ell}(u)\right) du \quad (12),$$

where f is any given function.

When the temperatures or the relative concentrations vary from a self-shielding region to another, we will use to integrate a function f_α defined on region α (for example the flux in that region), the quadrature formulas corresponding to the microscopic total cross section of the resonant mixture and to the microscopic partial cross-section of each component of the mixture in region α .

The code CALENDF [4] calculates quadrature formulas allowing us to integrate either any function f depending on lethargy u only through the total microscopic cross-section of a given isotope or the product of such a function f by any partial cross-section of this isotope. Here, we carry out such quadrature formulas by choosing as total microscopic cross-section the one of the mixture:

$$\sigma_0(u) = \sum_{m=1}^M a_{0m} \sigma_{0m}(u),$$

and as partial cross-section $[a_{0m} \sigma_{\rho 0m}(u)]$, where ρ is any partial cross-section.

If we note the group g probability table by $(p_i, \sigma_{ai,m}, \sigma_{si,m}, \sigma_i)_{m=1,M; i=1,N}$, we obtain the following quadrature formulas:

$$\frac{1}{\Delta u^g} \int_g \sigma_{s0m}(u) f(\sigma_0(u)) du \approx \frac{1}{a_{0m}} \sum_{i=1}^N p_i \sigma_{si,m} f(\sigma_i),$$

$$\frac{1}{\Delta u^g} \int_g \sigma_{a0m}(u) f(\sigma_0(u)) du \approx \frac{1}{a_{0m}} \sum_{i=1}^N p_i \sigma_{ai,m} f(\sigma_i).$$

3 Validation

To conclude we give two applications, the first one dealing with a homogeneous-medium source calculation and the second one with a UO₂ cell calculation without leakage. The multigroup mesh for APOLLO2 is the 172-group XMAS mesh. For each application, two APOLLO2 calculations were realized, the first one without the new mixture treatment (iterative method with 3 iterations) and the second one with the new mixture treatment.

3.1 Homogeneous medium

We took a homogeneous medium with 80% of uranium 238, 20% of uranium 235 and hydrogen at 300K and we carried out a source calculation. We compare the uranium 238 and 235 absorption rates versus a Monte-Carlo reference calculation performed with TRIPOLI4. [5] The new mixture treatment was applied between the groups 52 and 92 (2249 eV to 4. eV). The results are given in Figure 1.

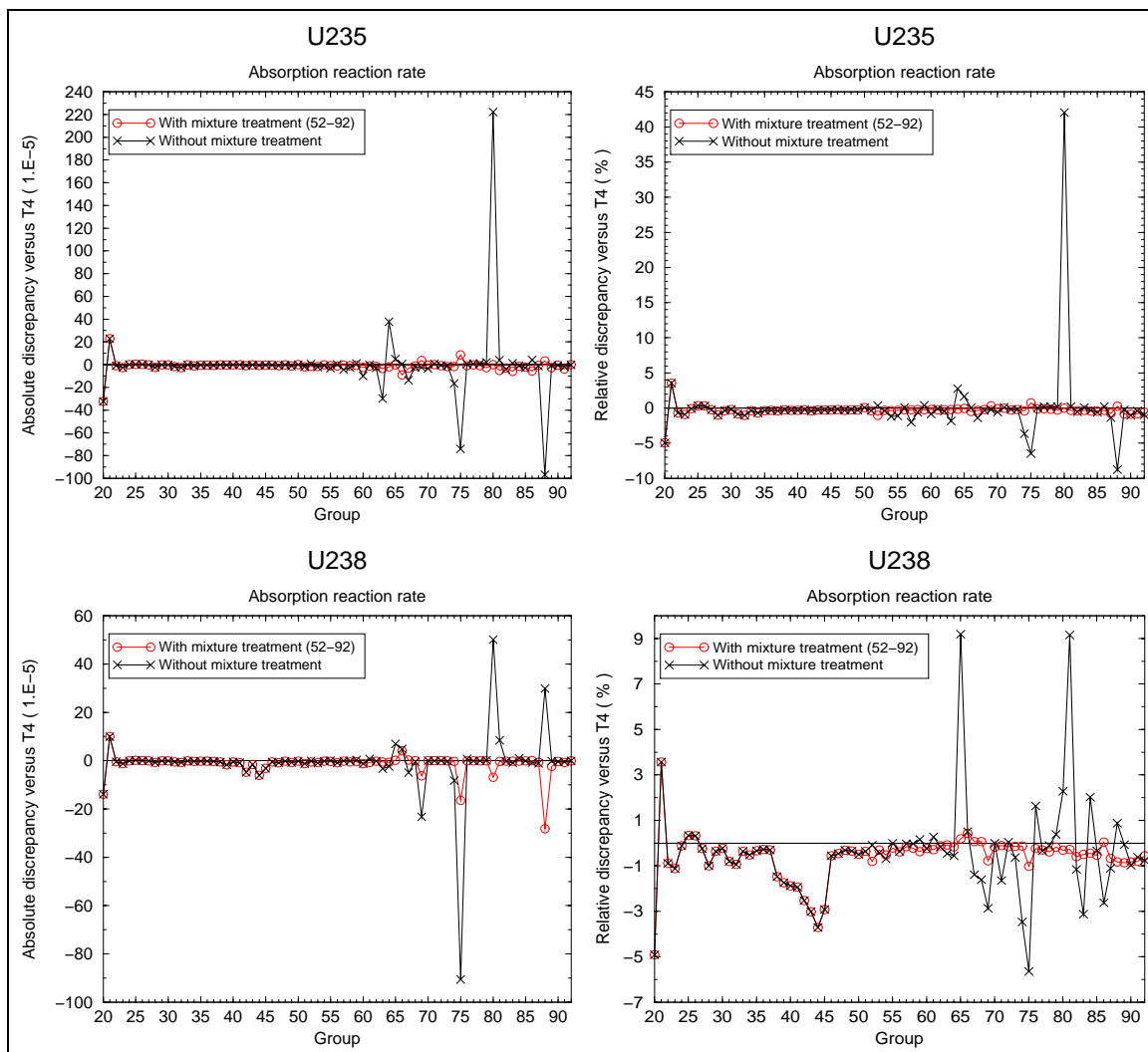


Figure 1: Absorption rate discrepancies in a homogeneous medium

In group 80 where there is a resonance overlapping between the resonances of uranium 235 and the 20.872 eV uranium 238 resonance, the discrepancies on the uranium 235 absorption

rate are reduced from 42.10% to 0.01% and the discrepancies on the uranium 238 absorption rate are reduced from 2.28% to (-0.31)%. We can also note a significant improvement for uranium 235 and 238 in group 75 (36.68 eV uranium 238 resonance) and for uranium 235 in group 88 (6.67 eV uranium 238 resonance). For uranium 238 in this group the two APOLLO2 results are almost the same but with opposite signs.

3.2 UO₂ cell

The second calculation was a cold UO₂ cell calculation without leakage with a uranium 235 enrichment of 3.7%. Here, we compare the effective multiplication factor and the uranium 238 and the uranium 235 absorption rates in the fuel to reference results given by an APOLLO2 calculation performed on a very fine multigroup mesh [6] (~12000 groups). The new mixture treatment was applied from group 74 to group 82 (40.17 eV to 13.71 eV).

The results concerning the reaction rates are given in Figure 2.

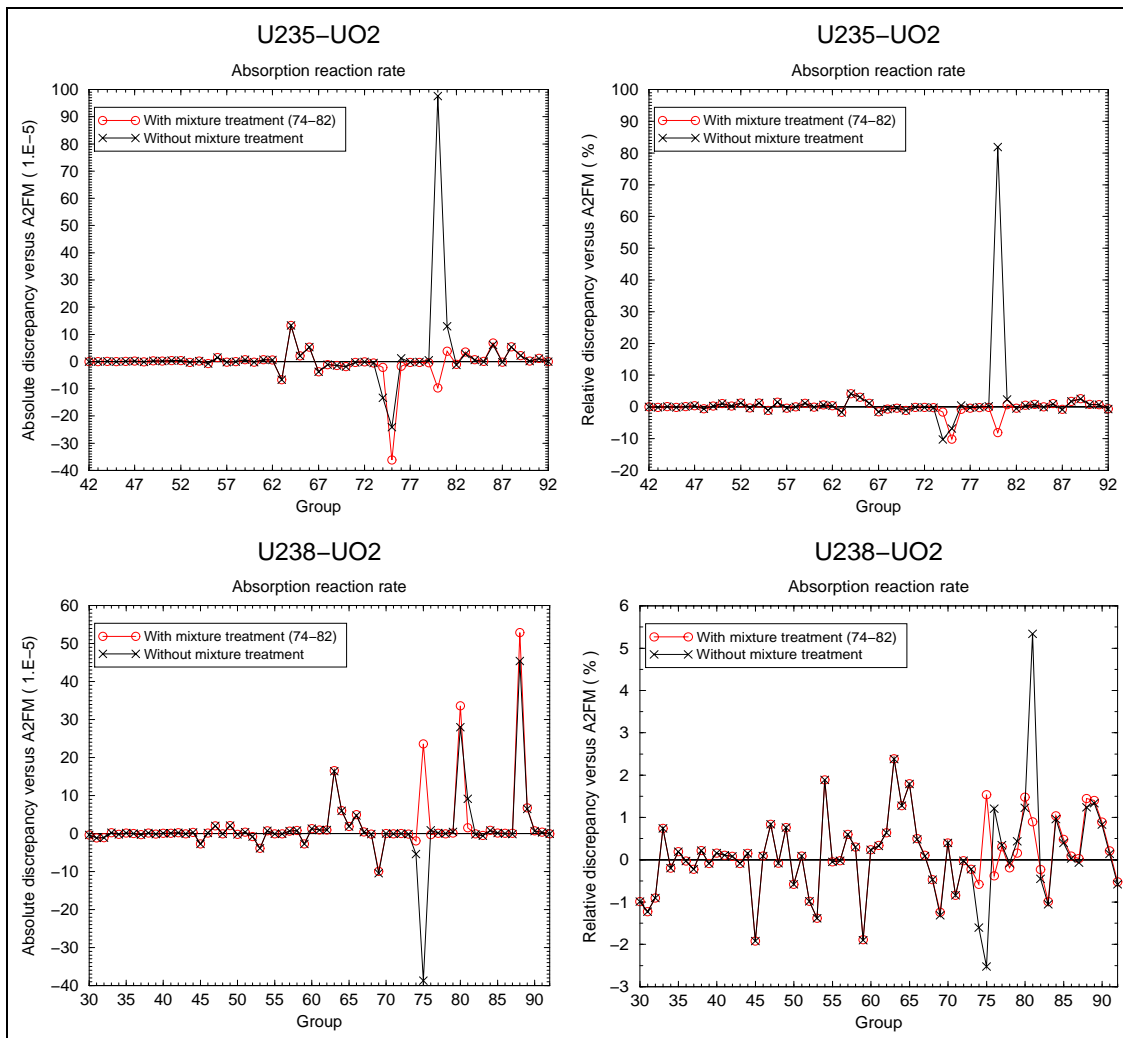


Figure 2: Absorption rate discrepancies in a UO₂ cell

With the mixture treatment, in group 80, the discrepancies on uranium 235 absorption rate are reduced from 81.85% to (-8.13)% and for uranium 238, the results are nearly the same: 1.23% or 1.48%. In group 75, the results are slightly worsened for uranium 235, from (-6.78)% to (-10.19)% and slightly improved for uranium 238, from (-2.52)% to 1.54%. Globally the re-

action rate calculation is improved, but the new mixture treatment suppresses compensation between the reaction rate discrepancies. That leads to a little greater discrepancy on the effective multiplication factor. The results are given in Table 1.

Reference calculation	Iterative treatment	New treatment
1.34552	1.34398	1.34343
	$\Delta = -154 \cdot 10^{-5}$	$\Delta = -209 \cdot 10^{-5}$

Table 1: Effective multiplication factor

4 Conclusion

These first results are very encouraging because we are now able to reduce reaction rate discrepancies that were very significant. Moreover, this new mixture treatment is very general and can be applied to a mixture with any number of components. A MOX cell calculation is in progress.

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6 References

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