RZ calculations for selfshielded multigroup cross sections

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Abstract

A collision probability method has been implemented for RZ geometries. The method accounts for white albedo, specular and translation boundary condition on the top and bottom surfaces of the geometry and for a white albedo condition on the outer radial surface. We have applied the RZ CP method to the calculation of multigroup selfshielded cross sections for Gadolinia absorbers in BWRs.

1. Aim of this work

Traditional depletion calculations of BWRs or PWRs cores use parameterized cross section data that are generated from detailed two-dimensional assembly transport calculations. Recently, gray Gadolinia fuel pins have been introduced in BWR assemblies as burnup absorbers. [1] These pins contain alternative pellets of UOX fuel and of UOX mixed with Gadolinia and, therefore, question the pertinence of the two-dimensional assembly calculations. Even though one will retain the scheme based on two-dimensional assembly calculations, which is mandatory to keep realistic computational times, a problem arises as to how to compute the required multigroup selfshielded cross sections for the gray Gadolinia pins. If the RZ effect is important, then selfshielding should be done in RZ geometry and equivalent selfshielded cross sections will have to be defined for use in the 2D transport assembly calculations.

Before investigating approximate selfshielding schemes, that may be based, for example, on one-dimensional calculations for the volume-averaged pin material or in separate one-dimensional selfshielding calculations for each one of the pellets, it is necessary to have a reference calculation that accounts for the true RZ structure of the gray pins. To this end we have developed a new RZ collision probability technique and implemented it in the APOLLO2 spectral assembly code. [2,3] As a first application we have run a RZ, k_∞ calculation for a cell with gray Gadolinia fuel with different selfshielding techniques and compared it with reference Monte Carlo results. Our results show that mixture interaction effects cannot be neglected.

For the illustration of the RZ shielding effect in a 2D fuel assembly we present the calculation of a BWR MOX assembly which is a modified test problem proposed in [4], where the original gadolinium bearing fuel pins are replaced by gray pins. After the selfshielding calculation on RZ motifs using different techniques, axially uniform cross sections for the XY assembly

calculation are obtained via the reaction rates preserving procedure. The results are compared with reference Monte Carlo results. The results show that the mixture interaction effects are less important in the two-dimensional assembly calculations. We remark that the approximate selfshielding technique, separate one-dimensional selfshielding calculation for each one of the pellets, gives the equivalent result to that of the RZ CP method. It could be a good choice for the routine industrial calculation.

2. Collision probability method for RZ geometries

We consider one-group transport with isotropic scattering in a heterogeneous domain D with boundary Γ. The domain is partitioned into a set of homogeneous regions that define on its boundary Γ a set of surfaces. We assume that the external sources are isotropic and uniform in each region and that neutrons enter the domain isotropically and uniformly through each surface. The formulation of the flat-flux collision probability method for general 3D geometries can be written as:

$$V_i\Phi_i = \sum_j P_{ij}F_j + \sum_\alpha I_{i\alpha}J^-_\alpha,$$

where the sums in j and α are, respectively, over all the regions in the domain and over all the surfaces on its boundary.

- V_i = volume or homogeneous region i,
- Φ_i = average flux in region i,
- P_{ij} = generalized collision probability from region j into region i,
- $F_i = \Sigma_{si}\Phi_i + S_i$ = average emission density in region i,
- $I_{i\alpha}$ = generalize 'incoming' probability from surface α into region i,
- J^-_α = current entering surface α.

Matrix coefficients P_{ij} and $I_{i\alpha}$ are computed via a numerical integration over the area $S_\perp(\mathbf{\Omega})$ transverse to the neutron trajectory:

$$P_{ij} = Kf_{ij},\ I_{i\alpha} = (4/A_\alpha)Kf_{i\alpha},$$

where K indicates the integration over the transverse plane and the f_{ij} and $f_{i\alpha}$ are analytical expressions to be evaluated over each of the numerical trajectories. For example, with τ_i the optical thickness across region i,

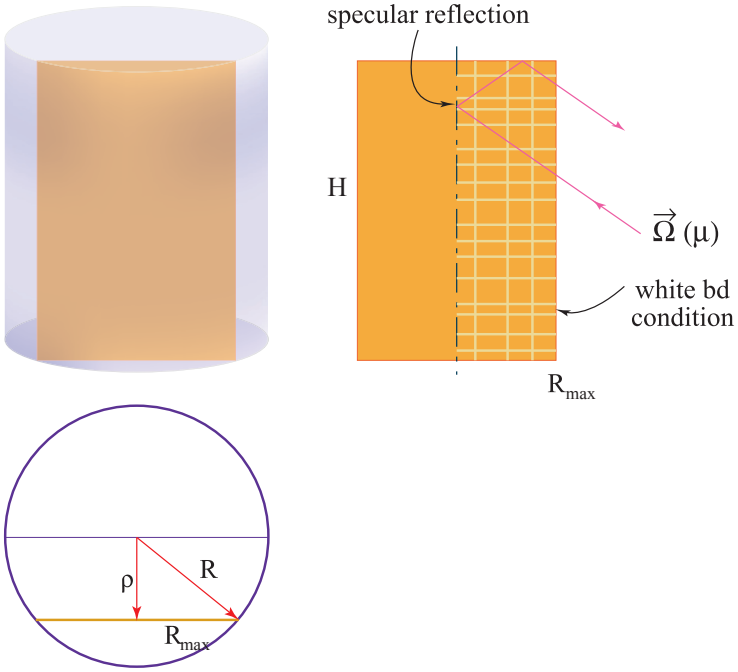
$$f_{ij} = \begin{cases} \frac{1-e^{-\tau_i}}{\Sigma_i}e^{-\tau_{ij}}\frac{1-e^{-\tau_j}}{\Sigma_j}, & i \neq j, \\ 2\frac{\tau_i-(1-e^{-\tau_i})}{\Sigma_i^2}, & i = j, \end{cases},$$

In 3D Cartesian coordinates, every trajectory is contained in a vertical plane. Therefore, the trajectory can be defined by the coordinates (ρ, φ) of the polar vector ρ orthogonal to the plane and by its local plane coordinates (z, θ). In these coordinates $d\mathbf{\Omega} = d\varphi \sin\theta d\theta$ and $dS_\perp = d\rho dz_\perp$ with $z_\perp = z\sin\theta$. For RZ geometries the integration over φ gives a factor π and we have

$$K_{RZ}f = \frac{1}{2}\int_0^R d\rho \int_0^\pi d\theta \sin\theta \int dz_\perp f(\rho,\theta,z_\perp). \sim \frac{1}{2}\sum_t w_t f(t),$$

the rightmost expression indicates that all the integrals are done by numerical discretization in ρ, θ and $z_\perp$. To generate the trajectories to each numerical ordinate ρ we compute the intersection of the geometric mesh with the corresponding vertical plane. As shown in Fig. 1 this reduces the problem to a series of two-dimensional trackings over a Cartesian mesh.

Figure 1: A radial quadrature abscissa defines a tangent plane where tracking in μ and $z_\perp$ has to be done. The figure shows the intersections of the RZ regions with the cut plane. A trajectory is shown for the case of specular reflection on the top boundary.

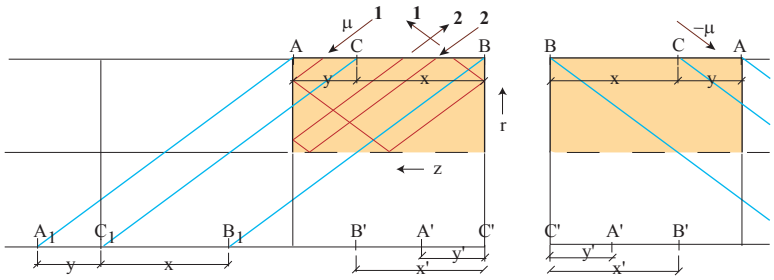


The main difficulty is the correct treatment of axial boundary conditions. In this work we have introduce compound trajectories. [5] This tracking technique ensures reciprocity and minimizes tracking storage and the subsequent numerical effort to compute the collision matrices. However, the tracking strategy is much more complicated that the one for single trajectories and depends on the type of geometrical motions applied as boundary conditions, in our case specular reflection and translation on the axial surfaces. The example in Fig. 2 illustrates the tracking technique.

3. Application to selfshielded multigroup cross section calculations

We have applied the newly developed collision probability method to RZ calculations of selfshielded cross sections for a cell containing a gray pin with radii .442 (pin), .5025 (clad) and .7306 (equivalent outer radius). The pin contains two pellets: a UOX pellet with 5%

Figure 2: Case with specular reflection on the top and bottom surfaces. To analyze the trajectories entering the free outer radial surface, the domain is extended by symmetries. The figure in the left shows the case for $\mu > 0$ when the number of domains between the farthest exiting point A_1 and the original domain is odd. By using symmetries to put back into the basic domain the exiting domain $A_1C_1B_1$ we find that trajectories entering via AC leave the domain with direction $-\mu$, while those entering via CB leave the domain via CB with (opposite) μ direction. The latter defines a mapping from CB into itself that maps a half of CB into the other half. Examples for these trajectories are shown as trajectories **1** and **2**. The right figure shows the tracking for direction $-\mu$.



enrichment in U235 (height 1 cm.) and a pellet with similar enrichment but with 5% in mass of Gadolinium (height .6 cm.). To account for skin effects we used 11 radial regions per pellet to define multigroup selfshielded cross sections for U238, U235 and the four resonant isotopes of Gadolinium: the innermost 9 regions have a volume equal to one tenth of the pellet volume, while the two more external regions have one twentieth of the volume each. The temperatures are: 627 (fuel), 327 (clad) and 300 (water) degrees C. Selfshielding and flux calculations were done with the APOLLO2 code and the 172-group (80 thermal) XMAS library.

The selfshielded cross sections were then used in a 2D RZ S_{16} cell calculation. As a comparison, we also computed selfshielded cross sections for each separate pellet in 1D cylindrical geometry. Table 1 compares the APOLLO2 results with a reference Monte Carlo calculation. [6] The results in the last row were obtained using the recently developed selfshielding formalism that accounts for interactions between mixed resonant isotopes. [7]

Table 1: Comparisons for k_∞ for a RZ cell with a gray Gadolinia pin. Reactivity error with respect to the TRIPOLI4 reference calculation.

mixture effects (pcm)	**RZ (a)**	**1D cells (b)**
without	-541	-506
with	-272	-454

(a) **RZ**: RZ selfshielding.
(b) **1D cells**: separate 1D selfshielding for each pellet.

Fig. 3 shows the group-by-group absorption errors from the RZ selfshielding with mixture effects with respect to the Monte Carlo reference. Table 2 gives a comparison for the errors for the absorption in two energy domains (macrogroups 1 to100 and 101 to 172) for the RZ selfshielding with and without mixture effects. We notice that accounting for resonance mixture

effects reduces the global macrogroup errors and, therefore, the error in reactivity.

Figure 3: Comparison with TRIPOLI4. Relative absorption errors (pcm) in the upper and lower pellets versus energy group.

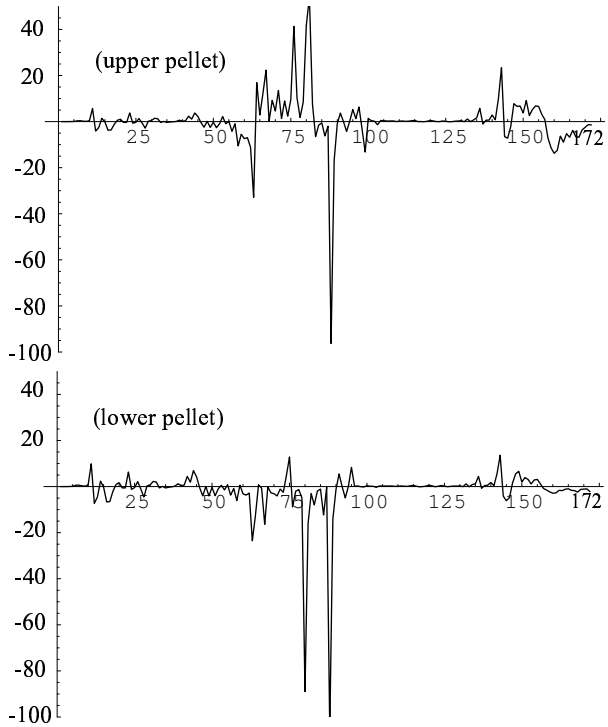


Table 2: Absorption errors in two energy domains (macrogroups 1 to100 and 101 to 172) for RZ selfshielding with and without mixture effects.

mixture effects (pcm)	upper pellet		lower pellet	
	1-100	101-172	1-100	101-172
without	-486	170	-300	88
with	56	-4	-329	24

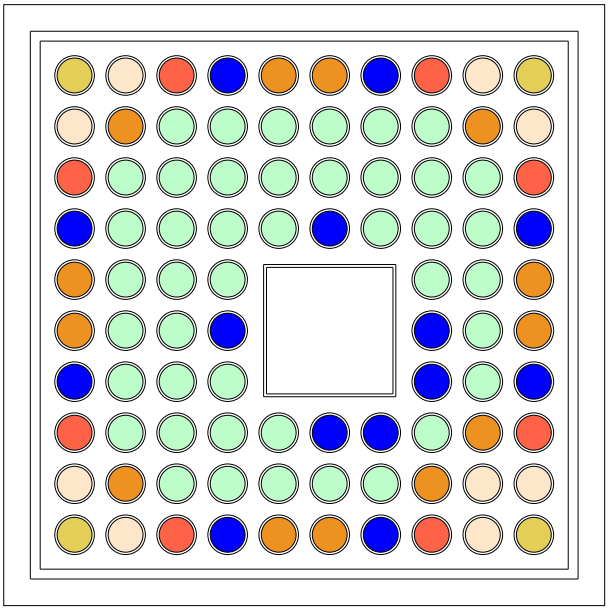
Clearly, these effects are important and should be accounted for in the calculation of multi-group selfshielded cross sections for gray Gadolinia pins. We did not observe appreciable effects when increasing the selfshielding mesh by halving axially each pellet.

4. Application to the BWR MOX assembly calculation

We have also applied the RZ collision probability method to the calculation of selfshielding cross sections of the gray Gadolinia pins in the BWR MOX assembly calculation. [4] Fig.4 shows the assembly geometry, the blue pins are replaced by the gray Gadolinia pins.

A pellet height of 1 cm is assumed and the gray pins are constructed by alternating one gadolinium bearing pellet and two UOX pellets. Radial dimensions, fuel compositions and

Figure 4: The BWR MOX assembly geometry.



temperatures of the gray pins are the same as in Section 3. The same radial division into 11 selfshielding regions is used in both pellets and the equivalent cross sections for the axially uniform pin in XY assembly calculation is represented by a set of 11 axially homogenized zones. The homogenization is done using the reaction rate preserving procedure in which the reference situation is represented by a RZ cylindrical cell surrounded by an assembly average buffer medium. The cross sections of buffer are obtained by flux weighting of a cell with an average assembly fuel. The reference flux in this RZ motif is calculated using the collision probability solver.

The selfshielding calculation is performed on a cylindrical RZ cell, as described in Section 3, both in RZ geometry and separately on two individual 1D cells. The selfshielded cross sections for the other pins are calculated taking into account the spatial interaction in a 2D XY configuration using a multicell UP1 option with 8 different cell types with 4 selfshielding regions each.

The selfshielded cross sections were then used in a 2D method of characteristics calculation. All the results were obtained using the selfshielding formalism that accounts for the interactions between mixed resonant isotopes. [7]

The reference calculation is provided by the Tripoli4 Monte Carlo Code [6] with an explicit geometrical description in 3D.

Table 3 compares the APOLLO2 reactivities with those of the reference Mont Carlo calculation. Table 4 shows the pin wise fission error bounds of the APOLLO2 results with respect to the Monte Carlo reference.

The results show that the RZ CP selfshielding is equivalent to the separate 1D selfshielding for each pellet in this BWR MOX assembly calculation.

5. Conclusion

We have presented a newly developed collision probability method for RZ geometries. We have applied the RZ CP method to the calculation of selfshielding cross sections for gray

Table 3: Comparison for k_∞ for a BWR MOX assembly. Reactivity errors with respect to the TRIPOLI4 reference calculation.

Reactivity errors (pcm)	Void fraction		
	0%	40%	70%
RZ (a)	-247	-228	-240
1D cells (b)	-250	-232	-247

(a) **RZ**: RZ selfshielding.
(b) **1D cells**: separate 1D selfshielding for each pellet.

Table 4: Comparison for fission rates for a BWR MOX assembly. Fission error bounds with respect to the TRIPOLI4 reference calculation.

Fission error bounds (%)	Void fraction								
	0%			40%			70%		
	Min	Max	RMS	Min	Max	RMS	Min	Max	RMS
RZ (a)	-1.1	1.2	0.5	-1.2	1.4	0.4	-1.3	1.3	0.6
1D cells (b)	-1.1	1.2	0.5	-1.2	1.4	0.4	-1.4	1.3	0.6

(a) **RZ**: RZ selfshielding.
(b) **1D cells**: separate 1D selfshielding for each pellet.

Gadolinia pins in BWRs. The results show that there is a non negligible effect in the approximate separate 1D selfshielding for each pellet scheme applied to a cell calculation, but the difference between the approximate scheme and the RZ selfshielding is vanishing when applied to our BWR MOX assembly calculation.

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