

HOMOGENIZATION OF LINEARLY ANISOTROPIC SCATTERING CROSS SECTIONS IN A CONSISTENT B_1 HETEROGENEOUS LEAKAGE MODEL

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ABSTRACT

One of the main problem encountered in cell calculations is that of spatial homogenization where one associates to a heterogeneous cell a homogeneous set of cross sections. The homogenization process is in fact trivial when a totally reflected cell without leakage is fully homogenized since it involved only a flux-volume weighting of the isotropic cross sections. When anisotropic leakages models are considered, in addition to homogenizing isotropic cross sections, the anisotropic scattering cross section must also be considered. The simple option, which consists of using the same homogenization procedure for both the isotropic and anisotropic components of the scattering cross section, leads to inconsistencies between the homogeneous and homogenized transport equation. Here we will present a method for homogenizing the anisotropic scattering cross sections that will resolve these inconsistencies.

I. INTRODUCTION

CANDU reactor calculations requires the knowledge of the few groups cell average macroscopic cross sections as well as the incremental cross sections associated with the reactivity control devices present in the core.^[1] The cell calculations required to generate the fuel average few group cross sections can generally be performed using an exact 2-D description of the cluster cell and a multigroup microscopic cross section library.^[2] The evaluation of the incremental cross sections associated with the reactivity devices on the other hand is generally based on a simplified 3-D supercell model where the fuel cells are partially homogenized and the reactivity control devices are located midway between two fuel channels. As a consequence, in addition to the full cell homogenization necessary to generate the fuel properties required in reactor core calculation, partial cell homogenization is also used before the 3-D supercell calculations are performed.

In the case where the heterogeneous cell transport calculations are performed in the absence of leakage, one can show that a flux-volume of homogenization on the main

transport cross section (total, fission and isotropic scattering) is sufficient to ensure that the total reaction rates obtained by solving the fully homogenized transport problem are identical to those computed using the heterogeneous transport solution. In the cases where a partial homogenization of the cell is considered, the equivalence between reaction rates is no longer ensured using this simple technique. However, it is possible to use various technique, including the SPH method, to redefine the partially homogenized cross sections in such a way as to restore the reaction rate equivalence relation between the two problems.^[3]

When the transport cell calculations are performed using an heterogeneous B_1 leakage model, an additional problem arises even if a full homogenization of the cell is considered.^[4, 5] Because this model involves the use of the linearly anisotropic component of the scattering cross section and result in the generation of directional currents in addition to the scalar flux, one needs to select an adequate homogenization technique for the anisotropic scattering cross section. One could use for instance the standard flux-volume homogenization. However, the problem with this technique is that the transport equation resulting from the homogenization process is incompatible with the equivalent homogeneous transport equation. Similarly, the use of a current-volume homogenization also leads to problem such as the fact one could use the buckling weighted average current and generate an homogeneous scattering cross sections or the directional currents to generate direction dependent scattering cross sections. However, as we will show in this paper, the equivalence between the homogeneous and homogenized transport problem is lost in both case.

One alternative to restore the equivalence between the two problems would be to use a method similar to the SPH technique. However, this would require the evaluation of SPH factor even in the case where a full cell homogenization is considered. Here we will use a different method which is based on the fact that by correcting adequately the fully homogenized anisotropic scattering cross section using the total cross section, the equivalence between the homogenized and homogeneous transport equation can be restored. We will also show that in the case where a partial homogenization of the cell is considered, this technique can also be used in a way which is compatible with the SHP method.

II. THE HETEROGENEOUS B_1 LEAKAGE MODEL

The multigroup transport equations which are solved in DRAGON when the heterogeneous B_1 leakage model is used are the following:^[4, 5]

$$V_i \Sigma_i^g \phi_i^g = \sum_{j=1}^N \left(Q_{0,j}^g(\phi) P_{ji}^g - \sum_{k=1}^3 B_k^2 V_j \psi_{j,k}^g P_{ji,k}^{g,*} \right) \quad (1)$$

$$V_i \Sigma_i^g \psi_{i,k}^g = \Lambda^g \sum_{j=1}^N \left(Q_{1,j,k}^g(\psi_k) + \frac{V_j \phi_j^g}{3} \right) P_{ji,k}^g \quad (2)$$

where we will have

$$Q_{0,j}^g(\phi) = V_j \sum_{h=1}^G \left(\Sigma_{0,j}^{h \rightarrow g} + \chi^g \nu \Sigma_{f,i}^h \right) \phi_j^h \quad (3)$$

$$Q_{1,j,k}^g(\psi_k) = V_j \sum_{h=1}^G \left(\Sigma_{1,i}^{h \rightarrow g} - \delta_{gh} \left[\frac{1 - \Lambda^h}{\Lambda^h} \right] (\Sigma_H^h - \Sigma_i^h) \right) \psi_{j,k}^h \quad (4)$$

and

$$\Sigma_H^g = \frac{\sum_j V_j \phi_j^g \Sigma_j^g}{\sum_j V_j \phi_j^g} \quad (5)$$

$$\delta_{gh} = \begin{cases} 1 & \text{for } g = h \\ 0 & \text{otherwise} \end{cases}$$

with Λ^g a function of B and Σ_H^g . Here $\Sigma_{1,i}^{h \rightarrow g}$ includes the $2l + 1 = 3$ term used in the spherical harmonic expansion of the scattering cross section and $\psi_{j,k}^g = j_{akk,j}^g$.^[4]

In the case of a totally reflected cell, the collision probabilities satisfy the following conservation relations:

$$\sum_{i=1}^N P_{ji}^g = 1 \quad (6)$$

$$\sum_{i=1}^N P_{ji,k}^{g,*} = 1 \quad (7)$$

$$\sum_{i=1}^N P_{ji,k}^g = 1 \quad (8)$$

III. FULL CELL HOMOGENIZATION

Let us first consider the case of an infinite and homogeneous cell. The above set of transport equations then becomes:

$$V \Sigma^g \phi^g = (Q_0^g(\phi) - B^2 V \psi^g) \quad (9)$$

$$V \Sigma^g \psi^g = \Lambda^g \left(Q_1^g(\psi) + \frac{V \phi^g}{3} \right) \quad (10)$$

where

$$Q_1^g(\psi) = V_j \sum_{h=1}^G (\Sigma_1^{h \rightarrow g}) \psi_j^h$$

since for an homogeneous cell $\Sigma_H^g = \Sigma_i^g$ and $\psi_k^g = \psi^g$ namely the current in every direction should be identical. We can also obtain the homogenized transport equations after summing Eqs. (1) and (2) over all the regions i :

$$V \Sigma_H^g \phi_H^g = \left(Q_{0,H}^g(\phi_H) - \sum_{k=1}^3 B_k^2 V \psi_{H,k}^g \right) \quad (11)$$

$$V\Sigma_{H,k}^g\psi_{H,k}^g = \Lambda^g \left(Q_{1,H,k}^g(\psi_{H,k}) + \frac{V\phi_H^g}{3} \right) \quad (12)$$

where we have used

$$V\phi_H^g = \sum_j V_j\phi_j^g,$$

$$V\psi_{H,k}^g = \sum_j V_j\psi_{j,k}^g$$

$$\Sigma_H^g = \frac{1}{V\phi_H^g} \sum_j V_j\phi_j^g\Sigma_j^g$$

$$\Sigma_{f,H}^g = \frac{1}{V\phi_H^g} \sum_j V_j\phi_j^g\Sigma_{f,j}^g$$

$$\Sigma_{0,H}^{h \rightarrow g} = \frac{1}{V\phi_H^h} \sum_j V_j\phi_j^h\Sigma_{0,j}^{h \rightarrow g}$$

$$\Sigma_{H,k}^g = \frac{1}{V\psi_{H,k}^g} \sum_j V_j\psi_{j,k}^g\Sigma_j^g$$

in such a way that

$$Q_{0,H}^g(\phi_H) = \sum_{h=1}^G \left(\Sigma_{0,H}^{h \rightarrow g} + \chi^g \nu \Sigma_{f,H}^h \right) V\phi_H^h$$

Now comparing Eqs. (9) and (11) we see that both equations are identical if one assumes that:

$$\phi = \phi_H$$

$$\psi = \frac{1}{B^2} \sum_{k=1}^3 B_k^2 \psi_{H,k}$$

$$Q_0^g(\phi) = Q_{0,H}^g(\phi_H)$$

and $\Sigma^g = \Sigma_H^g$. As a result, the flux-volume homogenization technique defined above for the various cross sections generates coherent flux equations.

For the current equations, the problem is not as straightforward. After some manipulations we can rewrite Eq. (12) as:

$$V\Sigma_H^g\psi_{H,k}^g = \Lambda^g \left(Q_{1,H,k}^g(\psi_{H,k}) + \frac{(\Sigma_H^g - \Sigma_{H,k}^g)}{\Lambda^g} V\psi_{H,k}^g + \frac{V\phi_H^g}{3} \right)$$

which can be transformed to a form identical to Eq. (10) using a B_k^2 weighted sum over the directional currents:

$$V\Sigma_H^g\psi_H^g = \Lambda^g \left(Q_{1,H}^g(\psi_H) + \frac{V\phi_H^g}{3} \right)$$

assuming

$$Q_{1,H}^g(\psi_H) = V \sum_{h=1}^G \left(\Sigma_{1,H}^{h \rightarrow g} - \delta_{gh} \left[\frac{1 - \Lambda^h}{\Lambda^h} \right] (\Sigma_H^h - \Sigma_H^h) \right) \psi_H^h = V \sum_{h=1}^G \Sigma_{1,H}^{h \rightarrow g} \psi_H^h$$

with

$$\Sigma_{1,H}^{h \rightarrow g} = \frac{1}{B^2 \psi_H^h} \sum_{j=1}^N \sum_{k=1}^3 \left(\Sigma_{1,j}^{h \rightarrow g} + \delta_{gh} (\Sigma_H^h - \Sigma_j^h) \right) B_k^2 \psi_{j,k}^h \quad (13)$$

As a result, one sees that the flux/volume homogenization of the anisotropic scattering cross sections should be replaced by the Eq. (13) to ensure that the homogenization process remains coherent.

IV. PARTIAL CELL HOMOGENIZATION

In the case where the cell resulting from the homogenization process is also heterogeneous, namely, the N initial regions are combined into M regions, each of these final regions I being composed of M_I initial regions i , then the M regions heterogeneous transport equations take the form:

$$V_I \Sigma_I^g \phi_I^g = \sum_{J=1}^M \left(Q_{0,J}^g(\phi_J) P_{JI}^g(\Sigma_I) - V_J \sum_{k=1}^3 B_k^2 \psi_{J,k}^g P_{JI,k}^{g,*}(\Sigma_I) \right) \quad (14)$$

$$V_I \Sigma_I^g \psi_{I,k}^g = \Lambda^g \sum_{J=1}^M \left(Q_{1,J}^g(\psi_{J,k}) + \frac{V_J \phi_J^g}{3} \right) P_{JI,k}^g(\Sigma_I) \quad (15)$$

where $P_{JI}(\Sigma_I)$ represents the fact that the collision probabilities are computed in this case using the homogenized cross sections Σ_I . The homogenized transport equation on the other hand takes the form:

$$\sum_{i \in M_I} V_i \Sigma_i^g \phi_i^g = \sum_{i \in M_I} \sum_{J=1}^M \sum_{j \in M_J} \left(Q_{0,j}^g(\phi_j) P_{ji}^g(\Sigma_i) - V_j \sum_{k=1}^3 B_k^2 \psi_{j,k}^g P_{ji,k}^{g,*}(\Sigma_i) \right) \quad (16)$$

$$\sum_{i \in M_I} V_i \Sigma_i^g \psi_{i,k}^g = \Lambda^g \sum_{i \in M_I} \sum_{J=1}^M \sum_{j \in M_J} \left(Q_{1,j}^g(\psi_{j,k}) + \frac{V_j \phi_j^g}{3} \right) P_{ji,k}^g(\Sigma_j) \quad (17)$$

The main problem here is that in order for Eqs. (14) and (16) to be equivalent we need:

$$\sum_{i \in M_I} V_i \Sigma_i^g \phi_i^g = V_I \Sigma_I^g \phi_I^g \quad (18)$$

$$Q_{0,J}^g(\phi_J) P_{JI}^g(\Sigma_I) = \sum_{i \in M_I} \sum_{j \in M_J} Q_{0,j}^g \phi_j P_{ji}^g(\Sigma_i) \quad (19)$$

and

$$V_J \sum_{k=1}^3 B_k^2 \psi_{J,k}^g P_{JI,k}^{g,*}(\Sigma_I) = \sum_{i \in M_I} \sum_{j \in M_J} V_j \sum_{k=1}^3 B_k^2 \psi_{j,k}^g P_{ji,k}^{g,*}(\Sigma_i) \quad (20)$$

to be simultaneously true. Because there is no simple relation between $P_{JI}^g(\Sigma_I)$ and $P_{ij}^g(\Sigma_j)$, the direct flux-volume homogenization method described in the previous section is no longer adequate. The alternative here is to use a non-linear process. Assuming that Eq. (18), which represents reaction rate conservation, is satisfied, we could redefine the homogenized flux and cross sections as follows:

$$\tilde{\phi}_I^g = \frac{1}{\mu_I^g} \phi_I^g \quad (21)$$

and

$$\tilde{\Sigma}_I^g = \mu_I^g \Sigma_I^g \quad (22)$$

where the factor μ_I^g are arbitrary and a flux-volume homogenization procedure similar to that used in the previous section was used for the flux ϕ_I^g and the cross section Σ_I^g (and $\Sigma_{f,I}^g$ or $\Sigma_{0,I}^{h \rightarrow g}$).

In the case where no leakage is present in the cell or the leakage is homogeneous, namely B_k^2 and $\psi_{j,k}^g$ are independent of the direction k , the SPH factors μ_I^g can be selected using an iterative process in such a way as to ensure that Eqs. (19) and (20) are satisfied simultaneously (since then $P_{ij,k}^g = P_{ij}^g/3$).^[3] As a result the currents will be homogenized using the relation:

$$\tilde{\psi}_{I,k}^g = \psi_{I,k}^g \quad (23)$$

which means that the total leakage rate out of the cell is conserved.

For the case where the heterogeneous B_1 leakage method is considered the problem is more complex since in addition to having directional collision probabilities which will make it difficult to satisfy Eqs. (19) and (20) the relation $P_{ij,k}^g = P_{ij}^g/3$ is no longer valid. Moreover, the current equation now becomes dependent on μ_I explicitly, namely Eq. (17) becomes:

$$V_I \tilde{\Sigma}_I^g \tilde{\psi}_{I,k}^g = \Lambda^g \sum_{J=1}^M \left(Q_{1,J}^g(\tilde{\psi}_{J,k}) + (\mu_I^g)^2 \frac{V_J \tilde{\phi}_J^g}{3} \right) P_{JI,k}^g(\tilde{\Sigma}_I) \quad (24)$$

As a result, obtaining the required SPH factor in this case would require an iterative solution of both current and flux solution.

However if we assume that for the homogenization process all the directional collision probability are identical and proportional to P_{ij}^g , and that Eq. (23) remains valid, then we can transform Eq. (24) to the form:

$$V_I \tilde{\Sigma}_I^g \tilde{\psi}_{I,k}^g = \Lambda^g \sum_{J=1}^M \left(\tilde{Q}_{1,J}^g(\tilde{\psi}_{J,k}) + \frac{V_J \tilde{\phi}_J^g}{3} \right) P_{JI,k}^g(\tilde{\Sigma}_I) \quad (25)$$

where

$$\tilde{\Sigma}_{1,I}^{h \rightarrow g} = \mu_I^h \Sigma_{1,I}^{h \rightarrow g} + \delta_{gh} \left((\mu_I^h)^2 - 1 \right) \frac{\tilde{\phi}_I^h}{\tilde{\psi}_I^h} \quad (26)$$

where $\Sigma_{1,I}^{h \rightarrow g}$ is homogenized using Eq. (13),

$$\tilde{\psi}_I^h = \frac{1}{B^2} \sum_{k=1}^3 B_k^2 \tilde{\psi}_{I,k}^h$$

and the standard SPH technique is still used to determine the factors μ_I^g .

V. RESULTS

We first tested the full homogenization technique in DRAGON for a simple cell problem with and without voiding.^[4] Three options have been considered. First, the standard flux-volume homogenization technique was used. Then, we considered an intermediate technique where Eq. (13) is replaced by

$$\Sigma_{1,H}^{g \rightarrow h} = \frac{1}{B^2 J_H^g} \int \sum_{k=1}^3 \Sigma_1^{g \rightarrow h}(\vec{r}) B_k^2 J_k^g(\vec{r}) d^3 r \quad (27)$$

namely, we assumed that the anisotropic scattering cross section is homogenized using a buckling weighted current-volume procedure. Finally we used the coherent homogenization process described above (see Eq. (13)).

The results we obtained for a full homogenization of these cells are presented in Table 1. The reference calculation represents the results obtained using a multiregion solution to the transport equation while for the three homogenized cases, a homogeneous cell was considered. Note that the radial, axial and total leakage computed are not affected considerably by the homogenization technique however, only the coherent homogenization technique ensure that the buckling eigenvalue is conserved after the cell homogenization. Moreover, this technique generates homogeneous diffusion coefficients which are identical to those obtained in the reference calculation while the two other homogenization techniques lead to errors which can reach 4 %.

The second problem we considered represents the partial homogenization to three regions and the condensation to 2 group of a CANDU 37-elements fuel cell. In this case the reference calculations were performed using the WIMS-Winfrith 69 groups library using the explicit cluster geometry where each of the 37 fuel pins are subdivided into 2 concentric annular regions while the coolant and moderator were subdivided respectively into 6 and 11 subregions. Using this reference solution, the macroscopic cross sections were first condensed to 2 energy groups the lower energy of the first energy group being located at 4 eV. For the three region homogenization we considered a fuel region which contain all the regions located inside the pressure tube (18 subregions), a calandria region which extends from the pressure to the calandria tube (3 subregions) and a unique moderator region (11 subregions). Using these homogenized and condensed cross sections we solved the resulting 3 region 2 group transport problem. In the case where the direct condensation is considered two options were studied, namely the original flux-volume homogenization and the coherent method described in Section III. We also considered the cases where the standard and modified (see Section IV) SPH homogenization technique were used. The results we obtained are presented in Table 2.

A few observations are immediately evident. The use of the SPH homogenization method improves substantially the value of the Buckling computed when the three region model is used. In fact, the correction term in B^2 introduced by the coherent homogenization method (-5 %) is much smaller than the correction term introduced by the SPH factors (-20 %). However, the diffusion coefficients are only marginally affected by the used of the SPH technique (1 %) while the difference observed between the flux-volume and the coherent homogenization technique is much larger (4 %) . In fact, the only homogenization technique which ensures that both the buckling and the diffusion

coefficient calculation are in agreement with the reference results is the combination of SPH+coherent method described in Section IV.

VI. CONCLUSION

As we saw above there exists a simple but coherent scheme that can be used for the full cell homogenization of the linearly anisotropic scattering cross sections in the heterogeneous B_1 leakage model. In the case where partial cell homogenization is considered we have shown that this coherent homogenization scheme can be combined with the SPH technique to generate an adequate homogenization procedure.

ACKNOWLEDGMENTS

This work was supported in part by a grant from the Natural Science and Engineering Research Council of Canada and by the CANDU Owner's Group.

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Table 1: Results of homogenization for the small cell model

Cell	Homogenization Model	B^2 (10^{-3} cm^2)	leakage rate (10^{-2} s^{-1})			D_H^g (cm)	
			radial	axial	total	$g = 1$	$g = 2$
Cooled	Reference	1.3333	3.920	1.965	5.885	1.135	0.507
	Flux-volume	1.3419	3.924	1.962	5.886	1.128	0.500
	Current-volume	1.3343	3.927	1.963	5.890	1.137	0.493
	Coherent	1.3333	3.923	1.962	5.885	1.135	0.507
Voided	Reference	-0.1885	-1.375	-0.704	-2.079	1.662	0.948
	Flux-volume	-0.1949	-1.386	-0.693	-2.079	1.608	0.916
	Current-volume	-0.1945	-1.386	-0.693	-2.079	1.612	0.908
	Coherent	-0.1885	-1.386	-0.693	-2.079	1.662	0.948

Table 2: Results for partial homogenization of the CANDU cell

Homogenization Model	B^2 (10^{-4} cm^2)	leakage rate (10^{-2} s^{-1})			D_H^g (cm)	
		radial	axial	total	$g = 1$	$g = 2$
Reference	3.0397	6.523	3.296	9.819	1.383	0.955
Flux-volume	3.8069	7.087	3.559	10.646	1.302	0.922
Coherent	3.6423	7.088	3.559	10.647	1.375	0.957
Flux-volume+SPH	3.1510	6.530	3.280	9.810	1.312	0.928
Coherent+SPH	3.0454	6.535	3.283	9.818	1.386	0.951