PHYSOR 2004 – The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, Illinois, April 25–29, 2004, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2004)

CANDU Adjuster Rods Incremental Cross Section Evaluation: A Perturbative Approach

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First order generalized perturbation theory can be used to evaluate the changes in integrated lattice parameters resulting from local variations in the lattice properties. Here such an approach is used to evaluate the incremental cross sections associated with the adjuster rods that can be inserted in a CANDU reactor. Comparisons with exact calculations show that the results obtained are reliable even if the perturbations are relatively large provided the reference unperturbed flux distribution is selected carefully.

KEYWORDS: perturbation theory, neutron transport, collision probability method, CANDU reactor

1. Introduction

Finite CANDU reactor calculations are generally performed in diffusion theory using the two-groups cell averaged fuel properties extracted from a two-dimensional lattice cell calculation. The effect of inserting structure materials and reactivity devices in the core is then simulated by adding to the fuel cell properties contributions in the form of incremental cross sections. Because the main reactivity control devices, including the adjuster rods, are positioned in a direction that is normal to the direction of the fuel channels, the required incremental cross sections cannot be evaluated using the two-dimensional transport model used for cell calculations. Accordingly, a more expensive three-dimensional supercell transport model must be considered [1]. Since the incremental cross sections are obtained by comparing the results from calculations with the control devices inserted and extracted from the supercell they represent good candidates for the application of a perturbation theory approach.

Perturbation theory methods were first introduced in reactor physics to evaluate the changes in the core multiplication constant resulting from variation in the cross sections [2]. Many years later, generalized perturbation theory (GPT) was suggested as a means to evaluate perturbatively variations in reaction rate ratios [3,4]. This approximation method was, and is still applied today with great success to problems involving the multigroup neutron diffusion equation [5,6]. Similarly, a large amount of effort has been dedicated to solving the adjoint transport equation using the Monte Carlo and discrete ordinates method. [7,8] More recently, a GPT approach has been

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implemented in DRAGON [9] for collision probability (CP) based transport calculations [10,11]. Here we propose to use this GPT approach to evaluate the incremental cross sections associated with adjuster rods.

In Section 2, we briefly review the generalized perturbation theory method and discuss its implementation in a CP based code. The general procedure required to evaluate the incremental cross sections associated with CANDU adjuster rods is presented in Section 3 while in Section 4 we discuss several options for the perturbative evaluation of the adjuster rods incremental cross section and analyze their respective performance. Finally in Section 5 we conclude.

2. Theoretical Background

Using the collision probability approximation, one can write the multigroup transport equation in the following matrix form: [11]

$$\mathbf{A}\vec{\phi} - \lambda\mathbf{F}\vec{\phi} = 0 \tag{1}$$

where

$$\mathbf{A} = \mathbf{I} - \mathbf{P}\boldsymbol{\Sigma_s}$$
$$\mathbf{F} = \mathbf{P}\boldsymbol{\chi}\left(\boldsymbol{\nu\Sigma_f}\right)^T = \mathbf{P}\boldsymbol{\Sigma_\lambda}$$

Here $\mathbf{P}$, the multigroup collision probability matrix with components

$$p_{ij}^g = \frac{1}{V^i}\int_{V_i} d^3r \int_{V_j} d^3r' \frac{e^{-\tau(|\vec{r}-\vec{r}'|,\vec{\Omega},\Sigma^g)}}{4\pi|\vec{r}-\vec{r}'|^2}$$

is full with respect to the regions and diagonal with respect to the groups. The scattering ($\boldsymbol{\Sigma_s}$) and production ($\boldsymbol{\Sigma_\lambda}$) matrices can both be written in the following block form:

$$\boldsymbol{\Sigma_{s/\lambda}} = \begin{pmatrix} \boldsymbol{\Sigma_{s/\lambda}}^{1\leftarrow 1} & \cdots & \boldsymbol{\Sigma_{s/\lambda}}^{1\leftarrow N_g} \\ \vdots & \ddots & \vdots \\ \boldsymbol{\Sigma_{s/\lambda}}^{N_g\leftarrow 1} & \cdots & \boldsymbol{\Sigma_{s/\lambda}}^{N_g\leftarrow N_g} \end{pmatrix}$$

where the diagonal sub-matrices $\boldsymbol{\Sigma_s}^{h\leftarrow g}$ and $\boldsymbol{\Sigma_\lambda}^{h\leftarrow g}$ are defined as:

$$\boldsymbol{\Sigma_s}^{h\leftarrow g} = \begin{pmatrix} \Sigma_{s,1}^{h\leftarrow g} & 0 & \cdots \\ 0 & \ddots & 0 \\ 0 & 0 & \Sigma_{s,N_i}^{h\leftarrow g} \end{pmatrix}$$
$$\boldsymbol{\Sigma_\lambda}^{h\leftarrow g} = \begin{pmatrix} \chi_1^h\nu\Sigma_{f,1}^g & 0 & \cdots \\ 0 & \ddots & 0 \\ 0 & 0 & \chi_{N_i}^h\nu\Sigma_{f,N_i}^g \end{pmatrix}$$

One can associate with the transport equation defined in Eq. (1) the following adjoint and generalized adjoint equations: [2,4]

$$\mathbf{A}^*\vec{\phi}^* - \lambda\mathbf{F}^*\vec{\phi}^* = 0 \tag{2}$$

$$\mathbf{A}^*\vec{\Gamma}^* - \lambda\mathbf{F}^*\vec{\Gamma}^* = \vec{S}^* \tag{3}$$

where:

$$\mathbf{A}^* = \mathbf{I} - (\boldsymbol{\Sigma_s})^T\,\mathbf{P}$$

$$\mathbf{F}^* = (\boldsymbol{\Sigma_\lambda})^T\,\mathbf{P}$$

and the generalized adjoint source $\vec{S}^*$ must be orthogonal with the flux.

Now let us assume that the matrices $\boldsymbol{\Sigma}$, $\boldsymbol{\Sigma_s}$ and $\boldsymbol{\Sigma_\lambda}$ are all perturbed due to a change in the cell properties. Such perturbations will be reflected by changes $\boldsymbol{\delta\mathbf{A}}$ and $\boldsymbol{\delta\mathbf{F}}$ in the transport operators. This then leads to perturbations $\boldsymbol{\delta\vec{\phi}}$ in the neutron flux and $\boldsymbol{\delta\lambda}$ in the eigenvalue. Assuming that the perturbations are small we can write [2,8]

$$\boldsymbol{\delta\lambda} \approx -\frac{\left\langle \vec{\phi}^*, \left(\boldsymbol{\lambda}\boldsymbol{\delta}\mathbf{F} - \boldsymbol{\delta}\mathbf{A}\right)\vec{\phi}\right\rangle}{\left\langle \vec{\phi}^*, \mathbf{F}\vec{\phi}\right\rangle} \tag{4}$$

where only first order contributions to $\boldsymbol{\delta\lambda}$ have been considered. Assuming we obtained a $\boldsymbol{G}$ group, $\boldsymbol{N}$ region solution $\vec{\phi}$ to the transport equation, one can define the group condensed and region averaged cross section $\boldsymbol{\Sigma^H_{x,J}}$ as:

$$\boldsymbol{\Sigma^H_{x,J}} = \frac{\sum_{i\in J}\sum_{g\in H}\boldsymbol{V_i}\boldsymbol{\phi^g_i}\boldsymbol{\Sigma^g_{x,i}}}{\sum_{i\in J}\sum_{g\in H}\boldsymbol{V_i}\boldsymbol{\phi^g_i}} = \frac{\left\langle \mathbf{M^H_J}\left(\Sigma_x\right)^T\vec{1}, \vec{\phi}\right\rangle}{\left\langle \mathbf{M^H_J}\vec{1}, \vec{\phi}\right\rangle} \tag{5}$$

where for each condensed group $\boldsymbol{H}$ and homogenized region $\boldsymbol{J}$, the matrix $\mathbf{M^H_J}$ takes the form

$$\mathbf{M^H_J} = \begin{pmatrix} \boldsymbol{\kappa_{1,H}}\mathbf{M_J} & \mathbf{0} & \cdots \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{\kappa_{G,H}}\mathbf{M_J} \end{pmatrix}$$

with:

$$\mathbf{M_J} = \begin{pmatrix} \boldsymbol{\kappa_{1,J}} & \mathbf{0} & \cdots \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \boldsymbol{\kappa_{N,J}} \end{pmatrix}$$

Here, $\boldsymbol{\kappa_{g,H}} = \mathbf{1}$ ($\boldsymbol{\kappa_{i,J}} = \mathbf{1}$) if group $\boldsymbol{g}$ (region $\boldsymbol{i}$) is included in condensation group $\boldsymbol{H}$ (homogenized region $\boldsymbol{J}$) and vanishes otherwise.

We can then approximate $\delta\Sigma^{H}_{x,J}$ using the following first order expression [8]

$$\delta\Sigma^{G}_{x,J} \approx \frac{\left\langle \mathrm{M}^{H}_{J}\left(\delta\Sigma_{x}\right)^{T}\vec{1},\vec{\phi}\right\rangle}{\left\langle \mathrm{M}^{H}_{J}\vec{1},\vec{\phi}\right\rangle} + \left\langle \vec{\Gamma}^{*},(\lambda\delta\mathbf{F}-\delta\mathbf{A})\vec{\phi}\right\rangle \tag{6}$$

where $\vec{\Gamma}^{*}$ is the solution to Eq. (3) with source:

$$\vec{S}^{*} = \frac{\mathrm{M}^{H}_{J}\left(\left(\Sigma_{x}\right)^{T}-\Sigma^{H}_{x,J}\mathrm{I}\right)\vec{1}}{\left\langle \mathrm{M}^{H}_{J}\vec{1},\vec{\phi}\right\rangle} \tag{7}$$

Here $\mathbf{I}$ is the identity matrix and $\Sigma^{H}_{x,J}$ is defined in Eq. (5).

Note that the term $(\lambda\delta\mathbf{F}-\delta\mathbf{A})$ can be approximated in a CP based code using:

$$(\lambda\delta\mathbf{F}-\delta\mathbf{A}) \approx \mathbf{P}(\Sigma)\left[\lambda\delta\Sigma_{\lambda}+\delta\Sigma_{s}-\delta\Sigma\right] \tag{8}$$

provided one considers only the leading order terms in the series expansion for the perturbed collision probabilities [11].

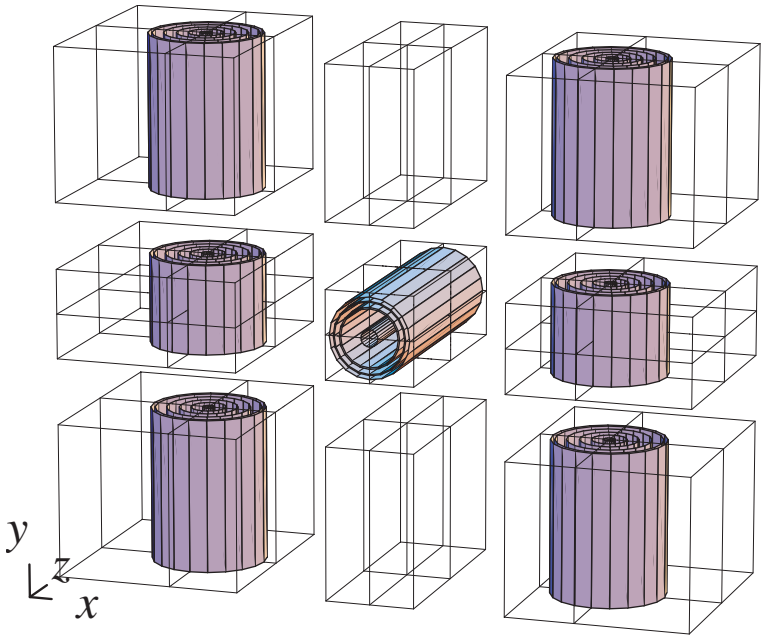

Fig. 1 DRAGON 3–D model for CANDU adjuster rod

3. Reference Calculations for CANDU Adjuster Rods

In CANDU reactor, the fuel channels run horizontally along the axis of the calandria (y axis). The adjuster rods are vertical tubes (in the z direction) that can be inserted in the core when required. They are located mid-way between two fuel

channels. The DRAGON model for the adjuster rods can be found in Figure 1. Here, one can first note that the fuel cluster has been annularized (see Figure 2). The second observation is that the rods themselves are made up of two concentric cylindrical regions containing stainless steel. These adjuster rods slide inside a perforated guide tube made up of a Zirconium alloy that is always present in the core. The adjuster rods come in six different types each being associated with different thicknesses of the stainless steel regions.

The general procedure that is used to evaluate the incremental cross section associated with the different types of adjuster rods and with the guide tube is the following. [1] One first perform a series of multigroup ($\boldsymbol{G}$ groups) two dimensional cell calculations to generate a multigroup cross-section data base for the fuel at mid-burnup. These cell properties are then homogenized as described in Figure 2 and the $\boldsymbol{G}$ groups macroscopic cross section associated with the resulting equivalent homogeneous mixtures are stored in a data base. As one can see, the 4 rings of fuel pins in the bundle are homogenized with some of the coolant to generate a set of four different mixtures each associated with an annular fuel region. The pressure tube, the gap and calandria tube are also homogenized to form a single pressure-to-calandria tube mixture. Note that since no group condensation is considered yet, the homogenization process will generate moderator properties that are identical to those used for the cell calculation itself. One must then add to the resulting macroscopic cross section

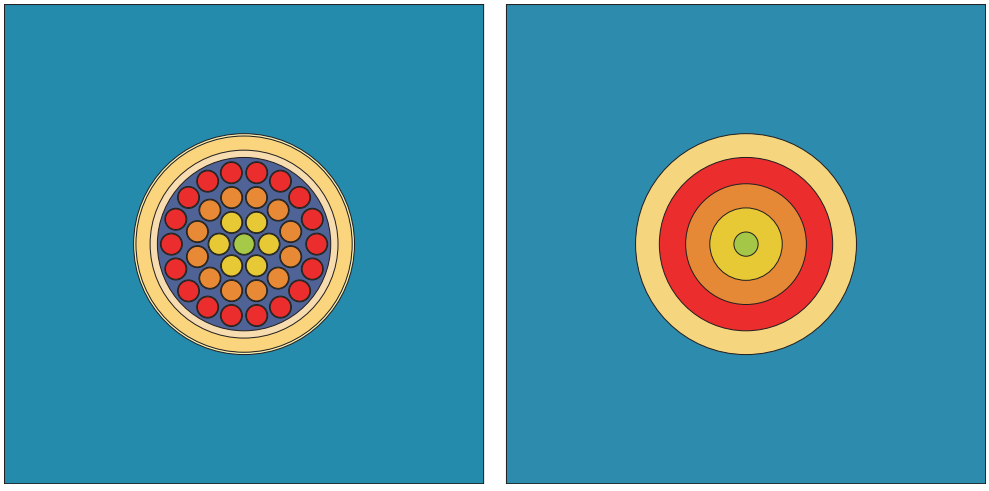

Fig. 2 2–D cluster model for CANDU fuel cell and homogenization model used in 3–D calculations

data base one mixture containing the stainless steel properties as well as a mixture of Zirconium and moderator that will be associated with the perforated guide tubes.

The second step consists in defining the three dimensional model that will be consider for incremental cross section evaluation. Here we selected a 3–D model where the fuel region is sub-divided into the four concentric cylinders defined by the cell homogenization problem. We also defined the adjuster rod geometry in the form of

concentric cylinders, the limits of these cylindrical regions matching those of the 6 types of adjusters. The final model we considered contains 512 regions. Typically, errors of the order of 5 % in the precision of the incremental cross section and k_{eff} are expected using such a model (note that the maximum change in k_{eff} or in the cross section resulting from the insertion of an adjuster is around 10%).

Eight successive 3–D supercell calculations must then be performed. First, a reference unrodded supercell calculation is performed. It consists in obtaining the cell-averaged properties for the case where both the guide tube and the adjuster rods are absent from the supercell. In order to compute the incremental cross section associated with the guide tube, a second supercell calculation is performed for the case where the annular region associated with the guide tube is now filled with the Zirconium/moderator mixture. Finally, the six different types of adjusters are modelled successively by replacing that various annular region initially containing moderator with stainless steel. Note that at the end of each of these supercell calculations, the cell properties are completely homogenized and the cross sections are condensed from G to 2 groups (lower energy limit of group 1 is 0.625 eV). The average CPU time for each supercell calculation is 19.5 minutes (for a total of 156 minutes for the 8 successive transport calculations) out of which 19 minutes are spent tracking the geometry and computing the multigroup collision probability matrix.

Table 1 Incremental cross section for the guide tube.

Property	Reference	Δ	δ
k_{eff}	1.05282855	-0.00385702	-0.36
Σ_a^1	0.00181611	0.00000421	0.23
$\nu\Sigma_f^1$	0.00087216	-0.00000087	-0.10
$\Sigma_s^{1\leftarrow 2}$	0.00006992	0.00000046	0.66
$\Sigma_s^{1\leftarrow 1}$	0.30394902	-0.00001022	0.00
Σ_a^2	0.00442027	0.00001586	0.36
$\nu\Sigma_f^2$	0.00519484	0.00000186	0.04
$\Sigma_s^{2\leftarrow 1}$	0.00863036	-0.00001898	-0.22
$\Sigma_s^{2\leftarrow 2}$	0.41941466	-0.00036883	-0.09

Assuming that the homogenized cross section associated with the unrodded supercell calculation are denoted $\Sigma_{x,U}$ and those associated with the guide tube are denoted $\Sigma_{x,G}$, the following values for the guide tubes incremental cross section $\Delta_{x,G}$ can be obtained

$$\Delta_{x,G}(\text{cm}^{-1}) = \Sigma_{x,G}(\text{cm}^{-1}) - \Sigma_{x,U}(\text{cm}^{-1}) \tag{9}$$

where the index x refers to different type of cross sections (including absorption, fission and scattering) as well as different groups. The change $\Delta_{k_{eff},G}$ in k_{eff} resulting

from the insertion of the guide tube can also be evaluated using

$$\Delta_{k_{eff},G} = (k^{G}_{eff} - k^{U}_{eff}) \tag{10}$$

where k^{U}_{eff} is the multiplication constant for the unrodded (reference) supercell and k^{G}_{eff} that for the supercell with the guide tube present. Similarly, for adjuster type I, we will have

$$\Delta_{x,I}(\mathrm{cm}^{-1}) = \Sigma_{x,I}(\mathrm{cm}^{-1}) - \Sigma_{x,U}(\mathrm{cm}^{-1}) \tag{11}$$

$$\Delta_{k_{eff},I}(mk) = (k^{I}_{eff} - k^{U}_{eff}) \tag{12}$$

Note that since the adjuster calculations are all performed assuming that the guide tube is present in the core, the incremental cross section computed in Eq. (11) also includes the effect of the guide tube given by Eq. (9).

The results we obtained for the incremental cross sections associated with the guide tube are presented in Table 1 where we have used

$$\delta_{x,G}(\%) = 100\frac{\Delta_{x,G}(\mathrm{cm}^{-1})}{\Sigma_{x,U}(\mathrm{cm}^{-1})}$$

$$\delta_{k_{eff},G}(\%) = 100\frac{\Delta_{k_{eff},G}}{k^{U}_{eff}}$$

One can also find in Table 2 the results for the change in the cell multiplication constant and in the cell averaged cross section sections due to the presence of each of the adjusters.

Table 2 Relative changes in supercell properties due to presence of adjuster rods

Property	δ(AR1)	δ(AR2)	δ(AR3)	δ(AR4)	δ(AR5)	δ(AR6)
k_{eff}	-5.55	-4.67	-8.28	-7.33	-3.42	-4.71
Σ^{1}_{a}	0.91	0.78	1.50	1.25	0.60	0.79
$\nu\Sigma^{1}_{f}$	-0.14	-0.13	-0.18	-0.17	-0.12	-0.13
$\Sigma^{1\leftarrow 2}_{s}$	7.49	6.27	11.60	10.12	4.58	6.33
$\Sigma^{1\leftarrow 1}_{s}$	0.16	0.13	0.31	0.24	0.08	0.13
Σ^{2}_{a}	6.70	5.58	10.37	9.07	4.02	5.64
$\nu\Sigma^{2}_{f}$	0.50	0.42	0.80	0.69	0.31	0.43
$\Sigma^{2\leftarrow 1}_{s}$	-0.45	-0.41	-0.65	-0.56	-0.34	-0.41
$\Sigma^{2\leftarrow 2}_{s}$	-0.06	-0.07	-0.04	-0.05	-0.07	-0.07

As one can see, the effect of the guide tube on core reactivity (-0.36 %) is relatively small compared to that of the adjuster rods (at least -3.42 %). Similarly the largest change in cross section due to the presence of the guide tube is only 0.36% (thermal absorption). This can be compared with the relatively large changes in the thermal absorption cross section that result from the insertion of an adjuster rod (4% for the weakest adjuster).

4. Perturbative Calculations for CANDU Adjuster Rods

Lets us first consider the evaluation of the incremental cross sections using our perturbative approach. In this case, one first performs a reference supercell calculation for the direct, adjoint and generalized adjoint flux for the unrodded supercell. Then the change in k_{eff} and in the two group cell averaged incremental cross section for the guide tube and the adjuster rods are evaluated using Eqs. (4) and (6). The results we obtained for the guide tube (GT) and the first adjuster rod (AR1) are presented in Table 3. For the guide tubes, ϵ is given by

$$\epsilon_x(\%) = 100\frac{|\Delta_{x,G} - \tilde{\Delta}_{x,G}|}{|\Delta_{x,G}|}$$

$$\epsilon_{k_{eff}}(mk) = 100\frac{|\Delta_{k_{eff},G} - \tilde{\Delta}_{k_{eff},G}|}{|\Delta_{k_{eff},G}|}$$

where $\tilde{\Delta}_{x,G}$ represents the variations in the incremental cross sections and k_{eff} computed using perturbation theory. Similar relations are also be used to compute ϵ for the adjuster rods.

Table 3 Perturbation theory errors (ϵ) based on unrodded supercell

Property	ϵ(GT)	ϵ(AR1)	ϵ(AR2)	ϵ(AR3)	ϵ(AR4)	ϵ(AR5)	ϵ(AR6)
k_{eff}	0.9	24.5	23.8	47.1	35.9	16.6	24.3
Σ_a^1	0.3	1.2	1.2	3.2	2.2	0.5	1.2
$\nu\Sigma_f^1$	0.9	3.7	3.3	8.3	6.1	2.2	3.4
$\Sigma_s^{1\leftarrow 2}$	0.3	22.9	22.1	47.1	34.9	14.9	22.6
$\Sigma_s^{1\leftarrow 1}$	2.0	0.5	0.5	1.4	0.9	0.2	0.5
Σ_a^2	0.9	26.3	25.3	53.6	39.7	17.5	25.9
$\nu\Sigma_f^2$	3.0	25.2	24.8	50.6	37.6	17.2	25.4
$\Sigma_s^{2\leftarrow 1}$	0.7	0.1	0.2	0.6	0.2	0.4	0.2
$\Sigma_s^{2\leftarrow 2}$	1.0	22.6	17.8	63.2	42.1	10.9	18.2

The first observation is that the perturbation theory results are very good for the guide tube but leads to relatively large errors for the adjuster rod itself. In fact, the changes in cross section resulting from the insertion of stainless steel tubes in the core are relatively large (much larger than the precision expected from the model) and the performance of the perturbation technique is, as expected, relatively poor. From the point of view of computation time, the total CPU time required for this calculation is 20 minutes. This is nearly 8 times faster than the CPU time required for the direct method.

Note that the choice of the reference for perturbative calculations is somewhat arbitrary. Even if selecting a unrodded supercell is adequate for the perturbative

Table 4 Perturbation theory errors (ϵ) based on adjuster 1 supercell

Property	ϵ(AR2)	ϵ(AR3)	ϵ(AR4)	ϵ(AR5)	ϵ(AR6)
k_{eff}	1.4	9.8	3.5	5.7	1.5
Σ_a^1	0.1	1.3	0.5	0.0	0.1
$\nu\Sigma_f^1$	0.4	1.3	0.3	1.0	0.4
$\Sigma_s^{1\leftarrow 2}$	1.3	10.1	3.5	5.1	1.4
$\Sigma_s^{1\leftarrow 1}$	0.1	0.7	0.2	0.2	0.1
Σ_a^2	1.5	11.1	3.9	6.0	1.6
$\nu\Sigma_f^2$	1.3	11.3	3.9	5.1	1.4
$\Sigma_s^{2\leftarrow 1}$	0.1	0.4	0.1	0.2	0.1
$\Sigma_s^{2\leftarrow 2}$	0.2	2.0	0.7	0.1	0.2

evaluation of the guide tube incremental cross section, this may not necessarily be the case when the adjusters are considered. One alternative is to select a more appropriate reference solution for the perturbative evaluation of the incremental cross section associated with the adjusters. From a physical point of view, one can consider all the adjusters as perturbations of a reference adjuster. Accordingly, one could use as the reference for our perturbative evaluation any one of the 6 adjusters including adjuster 1.

The results presented in Table 4 were obtained using the perturbative approach described in Section 2 but in this case the reference flux, adjoint and generalized adjoint correspond to a calculation with adjuster 1 inserted in the supercell. When comparing these results with those presented in Table 3 one observes substantial improvements in the results and most or our predictions now lies within the 5 % precision limit expected from the exact evaluation (except for AR3 where the errors can reach 10%). Optimizing the choice of the adjuster used as the basis for the perturbation calculation could possibly further improve these results.

Note that in this case, a second supercell calculation for the flux, the adjoint and the generalized adjoints must be performed. As a result, the total CPU time required for the analysis of the reference supercell, the guide tube and the six adjuster is 39.5 minutes. This still represents a gain of a factor of 4 in computation time as compared with the exact evaluation.

5 Conclusion

The GPT module implemented in DRAGON has been used to compute the incremental cross sections associated with CANDU adjuster rods and their associated guide tubes. In fact, the effect of the guide tube is sufficiently weak that the flux distribution inside an unrodded supercell can be used as the basis for a perturbation approach. On the other hand, this choice is not adequate when the effect of the adjuster on the supercell averaged cross sections required and a more adequate flux distribution must be selected. Here, by selecting the flux distribution associated with

adjuster 1 we were able to simulate the incremental cross section associated with the 5 other adjusters with errors reaching a maximum of 11.1 %. This compares very favorably with the 5 % error level associated with the supercell model. Optimizing the choice of the adjuster used as the basis for the perturbation calculation could possibly further improve these results.

For our best results, a gain of a factor of 4 in CPU time was observed. This gain looks small but is still appreciable for current CANDU applications. In addition, this technique is very promising for the design of new reactors concepts (Advanced CANDU reactors for example) where the exact composition and/or dimension of the control rods is not yet finalized.

Acknowledgments

This work was supported in part by a grant from the Natural Sciences and Engineering Research Council of Canada and by the Hydro-Québec chair in Nuclear Engineering.

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