GENERALIZED PERTURBATION THEORY IN DRAGON: APPLICATION TO PWR ASSEMBLY CALCULATIONS

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ABSTRACT

Generalized perturbation theory (GPT) is a mean to evaluate eigenvalue and reaction rates variations due to small changes in the lattice properties. It requires the evaluation of the changes in the neutron production and loss operators resulting from macroscopic cross sections variations. In fact these changes can be decomposed in two terms: a direct term for variations in source cross sections and an indirect term for the effect of total cross section variations on the collision probability (CP) matrix. As we will show, taking into account the direct term in a perturbation theory method is straight forward. However, a problem arises for CP matrix variation $\delta\mathbf{P_{VV}}$ since most of the computation effort is dedicated to the $\mathbf{P_{VV}}$ matrix calculation. This means that calculating $\delta\mathbf{P_{VV}}$ for each perturbation would annihilate the gains expected from using GPT. Here we will present a technique to replace the variation in $\mathbf{P_{VV}}$ by a source term variation. Comparison with exact perturbations will show that this approximation yields errors that can be neglected compared to the standard generalized perturbation theory errors. Results for temperature and fuel and water density perturbations on a 2D PWR 17x17 assembly will be presented.

1. INTRODUCTION

The first use of perturbation theory in neutronics was related to the computation of k_{eff} variations resulting from small changes in the cross sections (Davison, 1957). Later, Gandini introduced the generalized perturbation theory as a mean to evaluate variations in functionals of the flux such as reaction rates ratios (Gandini, 1967). In the code DRAGON, one can compute homogenized and group condensed properties

associated with an heterogeneous lattice (Marleau et al., 2000). This is achieved by solving the multigroup transport equation using the collision probability technique and then performing the required homogenization and condensation. Changes in material compositions (poison insertion or burnup) or local parameters (material temperatures or densities) yield perturbations in the cell properties. In such cases, a completely new flux solution is required to take into account the effect of the perturbations on the neutron flux.

Here, we propose to use a generalized perturbation theory method to produce an approximation of the perturbed homogenized and condensed cross sections without additional neutron flux calculations. In Section 2, we will briefly review the definition of the adjoint and generalized adjoint fluxes and how they can be computed in the code DRAGON.

Section 3 is devoted to the perturbation theory formulas. We will study the special case where there is no variation in the total cross section. Exact perturbation formulas and an approximation avoiding the computation of the perturbed collision probability matrix will also be presented.

In Section 4, we will present results for a PWR assembly and show that the proposed approximation has no effect on the accuracy of the method. Finally, we will conclude.

2. DIRECT AND ADJOINT FLUX COMPUTATION

Considering the collision probability formalism, the transport equation takes the form (Askew,1972):

$$\vec{\phi} = \mathbf{P}_{VV}\mathbf{R}_{\lambda}\vec{\phi} + \mathbf{P}_{VV}\vec{S} \tag{1}$$

where $\mathbf{P}_{VV}$ is the reduced collision probability matrix and:

$$\mathbf{R}_{\lambda} = \boldsymbol{\Sigma_s} + \lambda\boldsymbol{\chi\nu\Sigma_f}^{T} \tag{2}$$

is the neutron production matrix (including fission and diffusion). In the absence of any fixed source: $\vec{S} = \vec{0}$, λ is the eigenvalue of the problem ($\lambda = 1/k_{\mathit{eff}}$). If the fixed source does not vanish, $\lambda = 1$. Here, the flux $\vec{\phi}$ is a vector associated with a discretization over G energy groups and N regions. Its computation is based on a two level iterative scheme, the power iteration that deals with the fission source and the eigenvalue evaluation and the inner iteration that deals with the scattering sources (assuming a fixed fission source) (Marleau et al., 2000).

Once the flux is known, the homogenized and condensed properties over the heterogeneous lattice are obtained by:

$$G = \frac{1}{\bar{\phi}} \sum_{i=1}^{N} \sum_{g=1}^{G} \Sigma_i^g V_i \phi_i^g \tag{3}$$

with

$$\bar{\phi} = \sum_{i=1}^{N} \sum_{g=1}^{G} V_i \phi_i^g \tag{4}$$

where Σ_i^g is the cross section of interest (such as Σ, $\nu\Sigma_f$...) for the region i and the energy group g, and V_i is the volume for the region i. For simplicity we have considered in this paper a complete homogenization over the lattice and a condensation over all the energy groups. However, the method has been expanded to macro-region homogenization and few-group condensation. Equation (3) may be written in terms of a scalar product ratio:

$$G = \frac{\left\langle \vec{\Sigma}, \vec{\phi} \right\rangle}{\left\langle \vec{1}, \vec{\phi} \right\rangle} \tag{5}$$

One can associate with the direct eigenvalue transport equation (Eq. 1) an adjoint equation (Stacey, Jr., 1970):

$$\vec{\phi}^* = \mathbf{R}_\lambda^T \mathbf{P}_{\mathbf{VV}} \vec{\phi}^* \tag{6}$$

and to a given homogenized property G a generalized adjoint equation:

$$\vec{\Gamma}^* = \mathbf{R}_\lambda^T \mathbf{P}_{\mathbf{VV}} \vec{\Gamma}^* + \vec{S}^* \tag{7}$$

where $\vec{S}^*$ is computed by derivation with respect to the flux of the functional G:

$$\vec{S}^* = \frac{\vec{\Sigma}}{\left\langle \vec{1}, \vec{\phi} \right\rangle} - G \frac{\vec{1}}{\left\langle \vec{1}, \vec{\phi} \right\rangle} \tag{8}$$

The orthogonality between the direct flux and the generalized adjoint source:

$$\left\langle \vec{S}^*, \vec{\phi} \right\rangle = 0 \tag{9}$$

is imposed by the previous definition of $\vec{S}^*$. Such an othogonality is required to ensure that a solution for the generalized adjoint flux exists. In addition, $\vec{\Gamma}^*$ is chosen in such a way that it is orthogonal with the fission source:

$$\left\langle \vec{\Gamma}^*, \mathbf{P_{VV}} \boldsymbol{\chi\nu\Sigma_f}^T \vec{\phi} \right\rangle = 0 \tag{10}$$

In order to simplify the solution method for equations (6) and (7), we will introduce a pseudo-adjoint fux $\vec{\phi}^+$ and a pseudo-generalized adjoint flux $\vec{\Gamma}^+$ respectively defined by:

$$\vec{\phi}^+ = \mathbf{P_{VV}} \vec{\phi}^* \quad \text{and} \quad \vec{\Gamma}^+ = \mathbf{P_{VV}} \vec{\Gamma}^* \tag{11}$$

The pseudo-adjoint equations (associated with Eqs. 6 and 7) take the form:

$$\vec{\phi}^+ = \mathbf{P_{VV}} \mathbf{R}_\lambda^T \vec{\phi}^+ \tag{12}$$

$$\vec{\Gamma}^+ = \mathbf{P_{VV}} \mathbf{R}_\lambda^T \vec{\Gamma}^+ + \mathbf{P_{VV}} \vec{S}^* \tag{13}$$

Apart from the transposition of $\mathbf{R}_\lambda$, these equations are similar to the direct eigenvalue and fixed source equations (Eq. 1). The algorithms to compute the pseudo-adjoint and pseudo-generalized adjoint fluxes are very similar to the algorithm used for the direct flux calculation (Courau and Marleau, 2000). Once the pseudo fluxes have been computed, on can recover the adjoint and generalized adjoint fluxes using:

$$\vec{\phi}^* = \mathbf{R}_\lambda^T \vec{\phi}^+ \text{ and } \vec{\Gamma}^* = \mathbf{R}_\lambda^T \vec{\Gamma}^+ + \vec{S}^* \tag{14}$$

3. PERTURBATION THEORY AND COLLISION PROBABILITY METHOD

The direct transport equation (Eq. 1) may be written in the form (Stacey, Jr., 1970):

$$\mathbf{A}\vec{\phi} = \lambda \mathbf{F} \vec{\phi} \tag{15}$$

where

$$\mathbf{A} = \mathbf{I} - \mathbf{P_{VV}} \boldsymbol{\Sigma_s} \tag{16}$$

$$\mathbf{F} = \mathbf{P_{VV}} \boldsymbol{\chi\nu\Sigma_f}^T \tag{17}$$

$\mathbf{A}$ is the loss operator, $\mathbf{F}$ is the fission production operator. The associated adjoint and generalized adjoint equations take the form:

$$\mathbf{A}^* \vec{\phi}^* = \lambda \mathbf{F}^* \vec{\phi}^* \tag{18}$$

$$\left(\mathbf{A}^* - \lambda \mathbf{F}^*\right) \vec{\Gamma}^* = \vec{S}^* \tag{19}$$

with the orthogonality relation:

$$\left\langle \vec{\Gamma}^*, \mathbf{F}\vec{\phi} \right\rangle = 0 \tag{20}$$

Any perturbation of the reactor properties will result in a change of the operators $\mathbf{A}$ and $\mathbf{F}$:

$$\mathbf{A} \rightarrow \mathbf{A}_p = \mathbf{A} + \delta\mathbf{A} \tag{21}$$
$$\mathbf{F} \rightarrow \mathbf{F}_p = \mathbf{F} + \delta\mathbf{F} \tag{22}$$

To the perturbed operators, we will associate a perturbed flux solution and a perturbed eigenvalue:

$$\vec{\phi} \rightarrow \vec{\phi}_p = \vec{\phi} + \delta\vec{\phi} \tag{23}$$
$$\lambda \rightarrow \lambda_p = \lambda + \delta\lambda \tag{24}$$

The impact of $\delta\mathbf{A}$ and $\delta\mathbf{F}$ on the eigenvalue is given by the perturbation formula:

$$\delta\lambda^e = \frac{\left\langle \vec{\phi}^*, \left(\delta\mathbf{A} - \lambda\delta\mathbf{F}\right)\vec{\phi}_p \right\rangle}{\left\langle \vec{\phi}^*, \mathbf{F}_p\vec{\phi}_p \right\rangle} \tag{25}$$

This relation is formally exact and depends on the perturbed flux. Practically, the perturbed flux $\vec{\phi}_p$ is replaced by the reference flux $\vec{\phi}$ in the expression for $\delta\lambda^e$ to yield an approximate formula for $\delta\lambda$. Considering a functional G (Eq. 5), we have:

$$\delta G^e = \frac{\left\langle \delta\vec{\Sigma}, \vec{\phi}_p \right\rangle}{\left\langle \vec{1}, \vec{\phi}_p \right\rangle} + \frac{\left\langle \vec{1}, \vec{\phi} \right\rangle}{\left\langle \vec{1}, \vec{\phi}_p \right\rangle} \left\langle \vec{\Gamma}^*, \left(\delta\lambda\mathbf{F}_p + \lambda\delta\mathbf{F} - \delta\mathbf{A}\right)\vec{\phi}_p \right\rangle \tag{26}$$

This formula is also exact. We obtain an approximate relation for δG by replacing the perturbed flux by the reference flux. The exact formulations of $\delta\lambda^e$ and δG^e are of interest only in a validation phase. It is a good mean to evaluate the roundoff errors due to uncertainties on the flux and adjoint flux computations.

The operators $\mathbf{A}$ and $\mathbf{F}$ (eqs. 16 and 17) depend on the matrix $\mathbf{P_{VV}}$. To first order, any perturbation can be decomposed into two components:

- the first component involves the perturbation of the neutron production matrix $\mathbf{R}_\lambda$. In this case we have: $\delta\mathbf{A} = \mathbf{P_{VV}}\delta\mathbf{A}'$ and $\delta\mathbf{F} = \mathbf{P_{VV}}\delta\mathbf{F}'$.

- the second component involves the perturbation of $\mathbf{P_{VV}}$. The collision probability matrix depends on the total cross section:

$$\delta\mathbf{P_{VV}} = \mathbf{P_{VV}}(\Sigma + \delta\Sigma) - \mathbf{P_{VV}}(\Sigma). \tag{27}$$

Considering the special case where the matrix $\mathbf{P_{VV}}$ is stationary ($\delta\mathbf{P_{VV}} = 0$), it is possible to re-write the previous perturbation formulas in terms of pseudo-adjoint flux $\vec{\phi}^{+}$ and pseudo-generalized adjoint flux $\vec{\Gamma}^{+}$. We have:

$$\delta\lambda^{e} = \frac{\left\langle \vec{\phi}^{+}, \left(\delta\mathbf{A}' - \lambda\delta\mathbf{F}'\right)\vec{\phi}_{p} \right\rangle}{\left\langle \vec{\phi}^{+}, \mathbf{F}'_{p}\vec{\phi}_{p} \right\rangle} \tag{28}$$

and

$$\delta G^{e} = \frac{\left\langle \delta\vec{\Sigma}, \vec{\phi}_{p} \right\rangle}{\left\langle \vec{1}, \vec{\phi}_{p} \right\rangle} + \frac{\left\langle \vec{1}, \vec{\phi} \right\rangle}{\left\langle \vec{1}, \vec{\phi}_{p} \right\rangle} \left\langle \vec{\Gamma}^{+}, \left(\delta\lambda\mathbf{F}'_{p} + \lambda\delta\mathbf{F}' - \delta\mathbf{A}'\right)\vec{\phi}_{p} \right\rangle \tag{29}$$

where we used the following reciprocity relation for the CP matrix (Askew,1972):

$$\mathbf{V}\mathbf{P_{VV}} = \mathbf{P_{VV}}^{T}\mathbf{V} \tag{30}$$

and the operator $\mathbf{F}'_{p}$ is defined by: $\mathbf{F}'_{p} = \boldsymbol{\chi_{p}}\boldsymbol{\nu}\boldsymbol{\Sigma_{f_{p}}}$

In the general case, the component associated with $\delta\mathbf{P_{VV}}$ has to be computed. It is well known that in a flux computation, most of the computation effort is dedicated to the $\mathbf{P_{VV}}$ calculation. To minimize the computation work, the variation of the matrix $\mathbf{P_{VV}}$ due to a variation of the total cross section may be replaced by an equivalent source term variation (Macfarlane, 1992):

$$\delta\mathbf{P_{VV}}\mathbf{R}_{\lambda} \approx \mathbf{P_{VV}}\delta\boldsymbol{\Sigma} \tag{31}$$

Here, $\delta\boldsymbol{\Sigma}$ is analogous to a diagonal component of the scattering cross section matrix and is equal to the variation of the total cross section. This approximation is analogous to the transport correction. Considering a development in spherical harmonics of the flux, it does not take into account the effect of the perturbation on the high order components (Takahashi, 1966). As the equation (31) partially takes into account the variation of the matrix $\mathbf{P_{VV}}$, the expressions of $\delta\lambda^{a}$ and δG^{a} are approximated. This yields the following perturbation formulas:

$$\delta\lambda^{a} = \frac{\left\langle \vec{\phi}^{+}, \left(\left(\delta\mathbf{A}' + \delta\boldsymbol{\Sigma}\right) - \lambda\delta\mathbf{F}'\right)\vec{\phi}_{p} \right\rangle}{\left\langle \vec{\phi}^{+}, \mathbf{F}'_{p}\vec{\phi}_{p} \right\rangle} \tag{32}$$

and

$$\delta G^a = \frac{\left\langle \delta\vec{\Sigma}, \vec{\phi}_p \right\rangle}{\left\langle \vec{1}, \vec{\phi}_p \right\rangle} + \frac{\left\langle \vec{1}, \vec{\phi} \right\rangle}{\left\langle \vec{1}, \vec{\phi}_p \right\rangle} \left\langle \vec{\Gamma}^+, \left(\delta\lambda \mathbf{F}'_p + \lambda\delta\mathbf{F}' - (\delta\mathbf{A}' + \delta\mathbf{\Sigma})\right) \vec{\phi}_p \right\rangle \tag{33}$$

In order to qualify this method, we will evaluate different types of errors depending on the way the perturbed functionals are computed. To the reference state we may associate F, the reference functional $F = \{\lambda, G\}$. Considering the perturbed state, we have:

- the perturbed properties explicitly computed: $F \longrightarrow F_c$.
- the perturbed flux is used in the perturbation formula: $F \longrightarrow F_p$.
- the reference flux is used in the perturbation formula: $F \longrightarrow F_r$.

The relative variation is:

$$\delta F^c = \frac{F_c - F}{F} \tag{34}$$

To which the following errors can be associated:

$$\varepsilon_F^p = \tfrac{F_c - F_p}{F} \quad \text{and} \quad \varepsilon_F^r = \tfrac{F_c - F_r}{F} \tag{35}$$

Note that in the case where the $\mathbf{P_{VV}}$ matrix is stationary, ε_F^p is equal to the roundoff error associated with the flux and adjoint or generalized adjoint fluxes computations. In the general case ε_F^p also includes the errors due to the transfer of the total cross section. The error ε_F^r is the sum of the computation error and the errors due to the fact we have used the reference flux instead of the perturbed flux.

4. RESULTS AND ERROR ANALYSIS

In order to analyse the efficiency of the perturbation method implemented in the code DRAGON, we have studied the 2D PWR 17x17 assembly presented in figure 1 (Marleau et al., 2000). The calculations were performed using a 69-group cross sections taken from the WIMS-AECL Winfrith library (26 fast groups) (Donnelly, 1986). We were interested in showing that the transfer approximation (Eq. 31) had a negligible impact on the accuracy of the perturbation formulas. Then, using the transfer approximation we studied the effect of the water and fuel density perturbation on k_{eff} and $\nu\Sigma_f$ homogenized over all the assembly and condensed over all the energy groups.

Legend
Color by Mixture

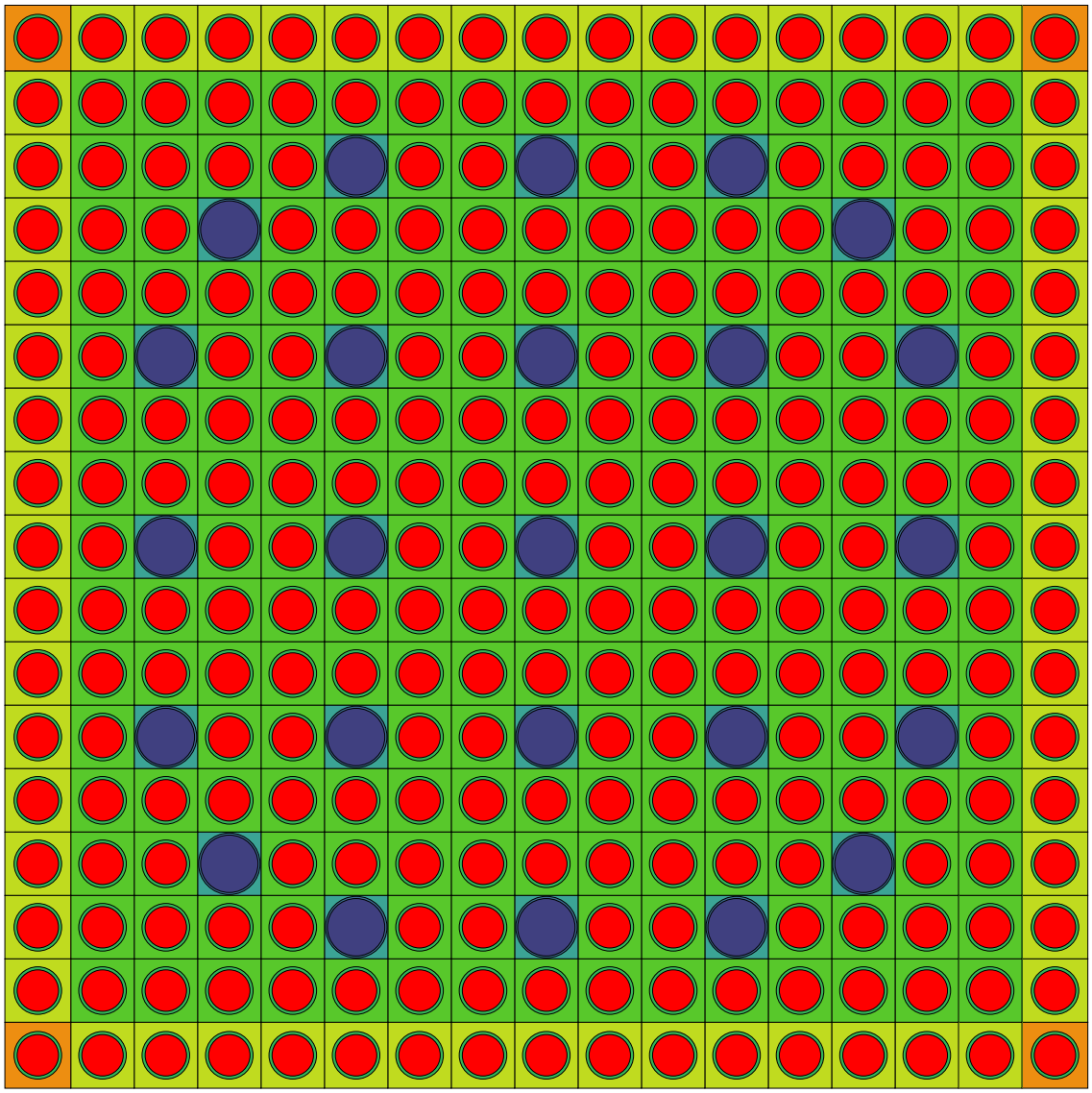

Figure 1 PWR 17x17 Assembly

(8)

4.1 Validation of the transfer approximation

To evaluate the impact of the transfer approximation we perturbed by a factor α the temperatures of the fuel and the moderator:

$$T_{f,0} = 933.6K \text{ and } T_{m,0} = 579.9K$$
$$T_f = (1-\alpha)T_{f,0} \text{ and } T_m = (1+\alpha)T_{m,0}$$

The integral properties computed are: k_{eff} and the homogenized and condensed production ($\nu\Sigma_f$), total (Σ) and scattering cross sections (Σ_s).

In order to evaluate the roundoff errors we have modified the perturbed state in such a way that the $\mathbf{P_{VV}}$ matrix is stationary. This was achieved by adding $\delta\Sigma$ to the perturbed transport correction. As we will see, the perturbed and modified perturbed states are slightly different. In this case, our point is to perform perturbations where $\mathbf{P_{VV}}$ is stationary. The table 1 presents the relative variation δF^c, the roundoff error ε_F^p and the standard error ε_F^r associated with the perturbation.

Table 1 Modified perturbed state

	α(%)	k_{eff}(pcm)	$\nu\Sigma_f$(%)	Σ(%)	Σ_s(%)
δF^c	5	84	-0.183	0.060	0.071
	10	173	-0.364	0.112	0.135
	20	364	-0.703	0.235	0.280
	50	1077	-1.505	0.597	0.706
ε_F^p	5	0	0.000	0.000	0.000
	10	0	0.000	0.000	0.000
	20	0	0.000	0.000	0.000
	50	0	0.000	0.000	0.000
ε_F^r	5	0	-0.004	0.001	0.002
	10	-2	-0.017	0.006	0.007
	20	-10	-0.067	0.022	0.025
	50	-62	-0.376	0.117	0.132

As one can see, α=50% leads to variations greater than 1000 pcm for k_{eff} and up to 1.5% for the homogenized and condensed cross sections which is above the small perturbation range. The roundoff error ε_F^p is $\leq$ 0.001% and therefore, may be neglected compared to the error ε_F^r. The standard error ε_F^r is quasi-quadratic in α which is in good agreement with the perturbation theory (Stacey, Jr., 1970).

In order to analyse the total cross section transfer approximation (Eq. 31), we have performed the same temperature perturbation but without modifying the transport correction. The table 2 presents the relative variation δF^c, the computation error ε_F^p and the standard error ε_F^r

The values associated with δF^c in the tables 1 and 2 are very similar. This shows that the transport correction modification has a low impact on the flux computation. The computation error ε_F^p which includes the errors due the cross section transfer approximation remains very low compared to the standard error ε_F^r. If we compare the standard errors presented in the tables 1 and 2, one can see that they are of the same order of magnitude. This implies that the transfer approximation does not deteriorate the accuracy of the method.

Table 2 Non-modified perturbed state

	α(%)	k_{eff}(pcm)	$\nu\Sigma_f$(%)	Σ(%)	Σ_s(%)
δF^c	5	84	-0.184	0.061	0.072
	10	171	-0.366	0.113	0.136
	20	362	-0.706	0.237	0.282
	50	1073	-1.511	0.599	0.708
ε_F^p	5	1	0.001	-0.001	-0.001
	10	1	0.002	-0.001	-0.001
	20	2	0.003	-0.002	-0.002
	50	4	0.005	-0.002	-0.003
ε_F^r	5	0	-0.003	0.001	0.001
	10	-1	-0.015	0.004	0.005
	20	-8	-0.064	0.020	0.023
	50	-58	-0.371	0.114	0.129

4.2 Fuel and water density perturbations

Using the same PWR assembly, we have perturbed the fuel and water mixture densities. We considered 5 parameters (α_i), the first four being associated with the density of the water in mixtures 1, 3, 5 and 6 and the last one with the density of U^{235} in mixture 8 (Fig. 1). First, each density d_i was perturbed independently by α_i: $d_{i,p} = (1+\alpha_i)d_i$ with $\alpha_i(\%) = \{1,2,5,10\}$. Afterward we considered 400 coupled perturbations where the densities were perturbed simultaneously with α_i chosen randomly between 0 and 10%. The figures 2 and 3 present the relative errors ε_F^r for k_{eff}(pcm) and $\nu\Sigma_f$(%) associated with the relative variation δF^c.

One can see that the errors are rather low, especially for λ, even if the perturbations are large (α_i=10%). Considering the coupled perturbation, they generally yield errors lower than the independent perturbations. These results show that the approximate generalized perturbation formulas implemented in DRAGON give a good estimate of the homogenized and condensed properties due to a change in the assembly properties.

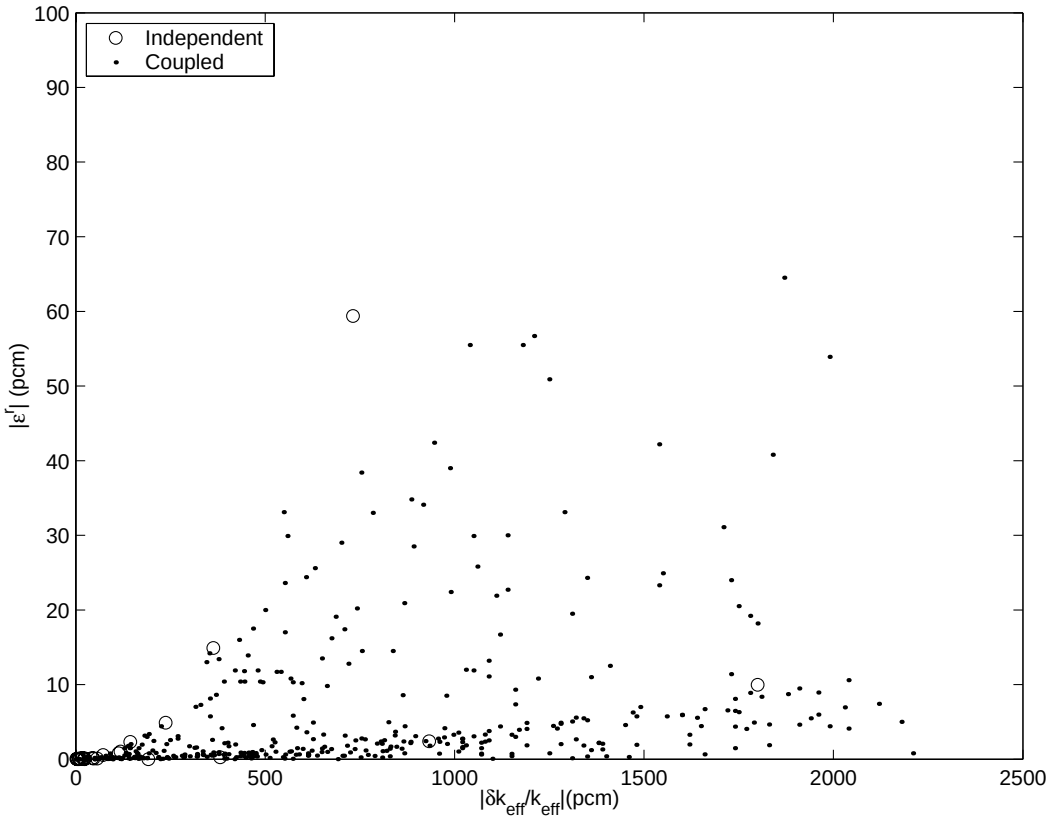

Figure 2 Relative error $|\varepsilon^r|$ versus relative variation for k_{eff}

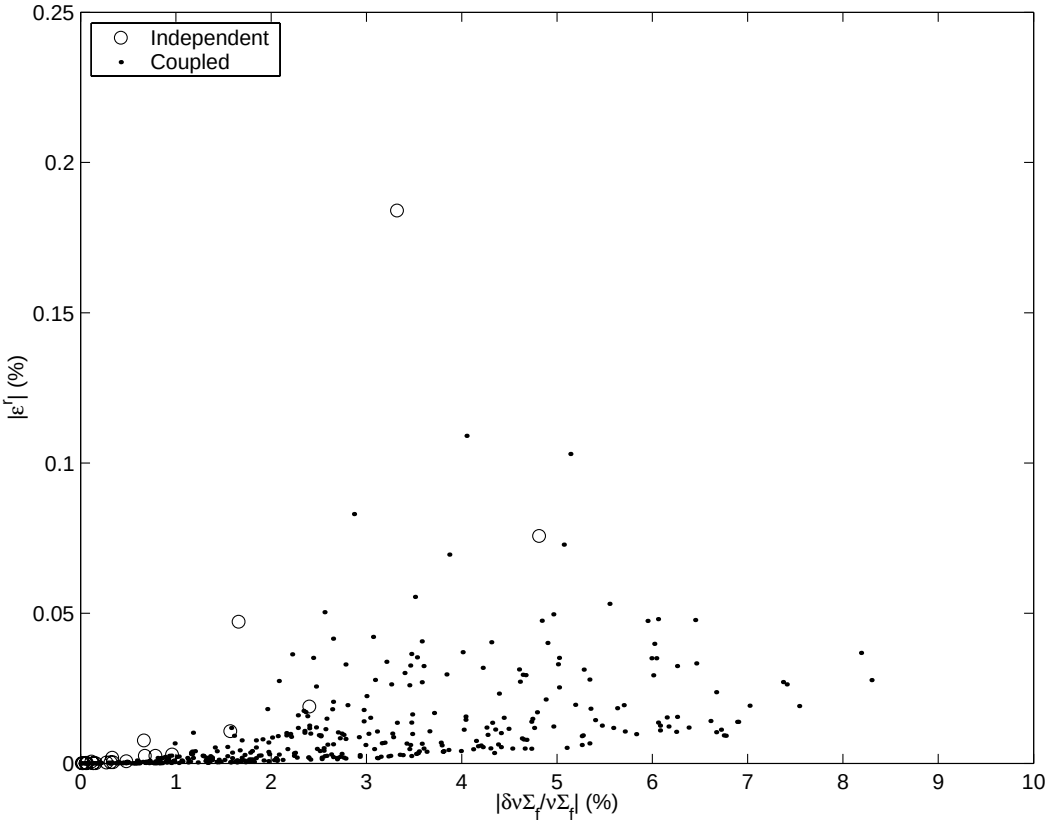

Figure 3 Relative error $|\varepsilon^r|$ versus relative variation for $\nu\Sigma_f$

5. CONCLUSIONS

In order to implement in the cell code DRAGON efficient GPT formulas, we proposed an approximation to bypass the perturbed collision probability matrix computation. For a PWR assembly the total cross section transfer (Eq. 31) approximation has a negligible impact on the errors associated with the standard generalized perturbation theory. The perturbation formulas implemented in DRAGON gave good results for a large range of perturbation. The computation of adjoint and generalized adjoint fluxes and the transfer approximation could be used to calculate reliable sensitivity coefficients associated with the homogenized and condensed properties.

For macro-region homogenization and few-group condensation problems, the computation of the generalized adjoint fluxes often presents difficulties associated with the structure of the generalized adjoint sources. A few modifications in the standard flux computation algorithm are required to ensure its efficiency and stability for the generalized adjoint flux calculation. For other type of lattices, such as CANDU cell, the approximation suggested in this paper may be less efficient. In that case, the computation of an additional correction term that would yield the same level of accuracy is being studied.

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