A PERTURBATION ANALYSIS SCHEME IN WIMS USING TRANSPORT THEORY FLUX SOLUTIONS

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ABSTRACT

Classical perturbation theory is widely used to calculate changes in reactivity due to variations in system parameters (e.g. material properties, reactor operating conditions, reactor geometry). This paper describes a new scheme to perform classical perturbation theory calculations that are based on transport theory flux solutions, through calculation of currents across all boundaries within a problem. This has been implemented in the reactor physics code WIMS. Group-wise sensitivity coefficients are evaluated using the perturbation methodology. For cases considered in this paper, excellent agreement was observed between WIMS and the Monte Carlo code MONK. Compared to use of diffusion theory, using transport theory was shown using a simple test case to give a more accurate breakdown of the change in reactivity because of a perturbation. This improved accuracy was due to a more accurate calculation of the leakage term.

Key Words: **perturbation, method of characteristics, transport theory, WIMS**

1. INTRODUCTION

Classical perturbation theory is widely used to calculate changes in reactivity due to variations in system parameters (e.g. material properties, reactor operating conditions, reactor geometry). In its first-order form, typical applications of this methodology are the calculation of sensitivity coefficients for use in uncertainty assessments and reactivity coefficients for use in kinetics studies. Other applications include the evaluation of localized (in terms of space and/or energy) responses to perturbations. Formulation of terms in the classical perturbation equation is dependent on the flux solution algorithm being used, specifically when considering the representation of neutron leakage. Whilst it is relatively straightforward to derive these terms in the context of diffusion theory, consideration of transport theory solution frameworks is more challenging.

This paper describes a new scheme to perform classical perturbation theory calculations that are based on transport theory flux solutions, by drawing analogies with diffusion-theory formulations. Whilst the new method is applicable to many transport theory algorithms (e.g. P_N, S_N), the focus of the work presented here is use of the method in conjunction with Method of Characteristics (MoC) solutions. Relative to diffusion-theory-based methodologies, it is expected that this new framework will provide improved accuracy in the estimation of quantities such as sensitivity coefficients in systems where transport theory effects are significant.

The scheme is one of a number of new uncertainty and sensitivity analysis tools currently being implemented in the WIMS reactor physics code suite [1], which is developed and marketed by the ANSWERS Software Service of Amec Foster Wheeler. Other tools that are currently being developed include facilities to assess the effects of manufacturing tolerances, geometric perturbations and the propagation of nuclear data uncertainties through burnup. Within WIMS, sensitivity coefficients calculated with the transport theory scheme can be combined with covariance data in order to assess overall calculation uncertainties.

The new transport theory scheme uses the diffusion-theory formulation as its starting point; this is described in the following section. The remainder of this paper describes the new method for use with transport theory flux solutions, as well as demonstration calculations with the new method.

2. APPLICATION OF CLASSICAL PERTURBATION THEORY WHEN USING DIFFUSION THEORY

The exact form of the classical perturbation equation can be expressed as

$$\delta k = \frac{\langle \phi^* | k\delta P - k\bar{k}\delta M | \phi \rangle}{\langle \phi^* | P | \phi \rangle} \quad (1)$$

where

- δk is the change in neutron multiplication factor due to the perturbation
- ϕ^* is the scalar adjoint flux in the perturbed system
- δP is the change in production rate due to the perturbation
- k is the neutron multiplication factor for the unperturbed system
- $\bar{k}$ is the neutron multiplication factor for the perturbed system
- δM represents the total change in absorption rates, scatter rates and leakage due to the perturbation
- ϕ is the scalar forward flux for the unperturbed system
- P is the production rate in the unperturbed system

The first-order form of Equation 1 assumes that both the forward and adjoint fluxes are calculated for the unperturbed system. Use of this approach enables the rapid calculation of δk for a large number of perturbed states, without having to perform a flux calculation for each of these perturbed states. This approach is typically used for generating sets of sensitivity coefficients where it can be assumed that the perturbations are small and do not lead to significant changes in the neutron spectrum in the system being considered. Equation 1 can be expanded in order to find the mesh-, group-, nuclide- and reaction-specific responses to a perturbation. For, example the absorption-specific contributions to Equation 1 can be calculated as

$$\frac{\langle \phi^* | k\bar{k}\delta A | \phi \rangle}{\langle \phi^* | P | \phi \rangle} = \frac{k\bar{k}\left(\sum_g \sum_x \sum_n V_x \bar{N}_n^x \bar{\sigma}_{a,n}^{x,g} \phi_x^g \phi^{*g}_x - \sum_g \sum_x \sum_n V_x N_n^x \sigma_{a,n}^{x,g} \phi_x^g \phi^{*g}_x\right)}{\langle \phi^* | P | \phi \rangle} \quad (2)$$

where

δA represents the total change in absorption rates due to the perturbation
g is an energy group index
x is a calculation mesh index
n is a nuclide index
V_x is the volume of calculation mesh x
N_n^x is the number density of nuclide n in calculation mesh x
$\sigma_{a,n}^{x,g}$ is the group g microscopic absorption cross-section of nuclide n in calculation mesh x

Barred quantities refer to those in the perturbed system.

When considering internal leakage terms (i.e. those terms representing leakage across internal surfaces of a model) in a diffusion theory solution it is assumed that the coupling coefficient between two adjacent meshes (1 and 2) can be represented as

$$D = \frac{(x_1 + x_2)D_1D_2}{x_1D_2 + x_2D_1} \tag{3}$$

where

x is the mesh width
D is the diffusion coefficient in the mesh

By assuming that the inter-mesh neutron current can be calculated as $-D\nabla\varphi$ and that diffusion coefficients can be calculated as $1/3\Sigma_{tr}$ (where Σ_{tr} is the macroscopic transport cross-section) it can be shown that the internal leakage components of Equation 1 can be estimated as

$$\frac{\langle\phi^*|k\bar{k}\delta L_{int}|\phi\rangle}{\langle\phi^*|P|\phi\rangle} = \frac{-k\bar{k}\left(\frac{\sum_g\sum_x\sum_n\sum_{s\in int}2S_s\phi_x^{*g}\left(\phi_x^g-\phi_s^g\right)\left[x_x\left(N_n^x\sigma_{tr,n}^{x,g}-\bar{N}_n^x\bar{\sigma}_{tr,n}^{x,g}\right)+x_s\left(N_n^s\sigma_{tr,n}^{s,g}-\bar{N}_n^s\bar{\sigma}_{tr,n}^{s,g}\right)\right]}{3\left(x_x\Sigma_{tr}^{x,g}+x_s\Sigma_{tr}^{s,g}\right)\left(x_x\bar{\Sigma}_{tr}^{x,g}+x_s\bar{\Sigma}_{tr}^{s,g}\right)}\right)}{\langle\phi^*|P|\phi\rangle} \tag{4}$$

where

δL_{int} represents the total change in internal leakage due to the perturbation
s is a direction index, corresponding to a surface which links to another calculation mesh
S_s is the surface area of surface S
$\sigma_{tr,n}^{x,g}$ is the group g microscopic transport cross-section of nuclide n in calculation mesh x
$\Sigma_{tr}^{x,g}$ is the group g macroscopic transport cross-section in calculation mesh x
x_i is the width of mesh i

When considering external leakage (i.e. leakage across external surfaces of a model) a typical "lambda" representation is adopted. Under this approach the neutron current across the edge of a model is assumed to be calculated such that $-D\nabla\phi = \lambda\phi$. Lambda provides a measure of the distance ($= D/\lambda$) from the model edge at which the flux becomes zero.

It can thus be shown that the external leakage components of Equation 1 are given by

$$\frac{\langle \phi^* | k\bar{k}\delta L_{ext} | \phi \rangle}{\langle \phi^* | P | \phi \rangle} = k\bar{k} \left(\frac{\sum_g \sum_x \sum_n \sum_{s \in ext} S_s \phi^{*g}_x \phi^g_x \left[N^x_n \sigma^{x,g}_{tr,n} \left(6\lambda\bar{\lambda}x_x - 4\lambda / \Sigma^{x,g}_{tr} \right) + \bar{N}^x_n \bar{\sigma}^{x,g}_{tr,n} \left(6\lambda\bar{\lambda}x_x - 4\bar{\lambda} / \bar{\Sigma}^{x,g}_{tr} \right) \right]}{\left(3\lambda x_x \Sigma^{x,g}_{tr} + 2\right)\left(3\bar{\lambda} x_x \bar{\Sigma}^{x,g}_{tr} + 2\right)} \right) \Bigg/ \langle \phi^* | P | \phi \rangle \tag{5}$$

where δL_{ext} represents the total change in internal leakage due to the perturbation

3. APPLICATION OF CLASSICAL PERTURBATION THEORY WHEN USING TRANSPORT THEORY

A challenge when deriving a form of the classical perturbation equation for use with transport theory flux solutions is how to treat the leakage terms. It is not always practical to extract leakage terms from a transport solution in a form that makes them suitable for use in perturbation analysis; particularly if it is required to break down the response to a perturbation into its constituent nuclide/reaction/group components.

A new methodology has been developed with the intention that it can applied to calculations performed with a range of transport theory solution schemes. The method assumes that the diffusion-theory forms of the leakage expressions (Equation 4 and Equation 5) can be adopted, but aims to correct the mesh coupling coefficients and lambda values for transport theory effects.

It is assumed that the transport solver being used is capable of calculating currents across all internal and external surfaces of a problem. On this basis, the effective inter-mesh coupling coefficients can be calculated as [2]

$$D_{eff} = -\frac{J_{transport}}{\nabla\phi_{transport}} \tag{6}$$

where both the current and flux gradient are calculated from a transport theory solution. By making the approximation that the leakage can be expressed according to Equation 6, it is thus possible to utilise the diffusion-theory form of the perturbation equation whilst using flux solutions from transport-theory solvers.

Multiplicative scaling factors are applied to the transport cross-sections, such that the inter-mesh coupling coefficients match the effective values calculated from Equation 6. The adjusted transport cross-sections are then used in Equation 4 and Equation 5.

Once a transport solution has been used to assess the currents across the external surfaces of a model, an effective value of lambda can be derived such that the transport-theory estimate of external leakage is reproduced in the diffusion-theory formulism. Such effective values of lambda are used in Equation 5.

4. DEMONSTRATION CALCULATIONS

4.1. Calculation of Uncertainties for a PWR Lattice

The WIMS code scheme has been used to assess k-infinity uncertainties due to microscopic cross-sections for a representative PWR lattice with reflective boundary conditions. The assumed assembly design for these calculations was UOX-1 from the KAIST benchmark (Figure 1) [3].

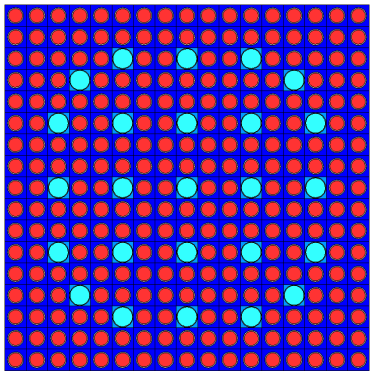

Figure 1. KAIST Benchmark model of a 17x17 PWR assembly

The first-order form of Equation 1 was used to calculate group-wise sensitivity coefficients within the WIMS code scheme. Flux calculations were performed with the CACTUS MoC solver. Sensitivity coefficients were evaluated for the change in k-infinity with respect to group-wise perturbations in the microscopic cross-sections for U235 fission, U235 capture and U235 nubar (average number of neutrons released per fission). Each calculation considered the perturbation of data in each of the 172 WIMS energy groups in turn. Sensitivity coefficients were calculated in each of these 172 energy groups and then combined linearly to form sensitivity coefficients in 44 energy groups (the group scheme used for the available covariance data).

The assumed form of the sensitivity coefficients was

$$S_g = \frac{\partial k}{\partial \sigma} \frac{\sigma_{0,g}}{k} \tag{7}$$

where $\sigma_{0,g}$ is the value of the group g unperturbed cross-section.

In all cases a perturbation size of 10% was assumed. The WIMS sensitivity coefficients were compared with equivalent values derived by MONK [4], which is a continuous-energy Monte Carlo code used for criticality and reactor physics analysis. Features within MONK facilitate the estimation of uncertainty on k-infinity due to nuclear data via a Differential Operator Sampling (DOS) formulation [5].

Plots of the WIMS and MONK estimates of sensitivity coefficients, as a function of energy, are shown in Figure 2, Figure 3 and Figure 4. It is observed that the sensitivity coefficients calculated by WIMS and MONK are in good agreement at all energies.

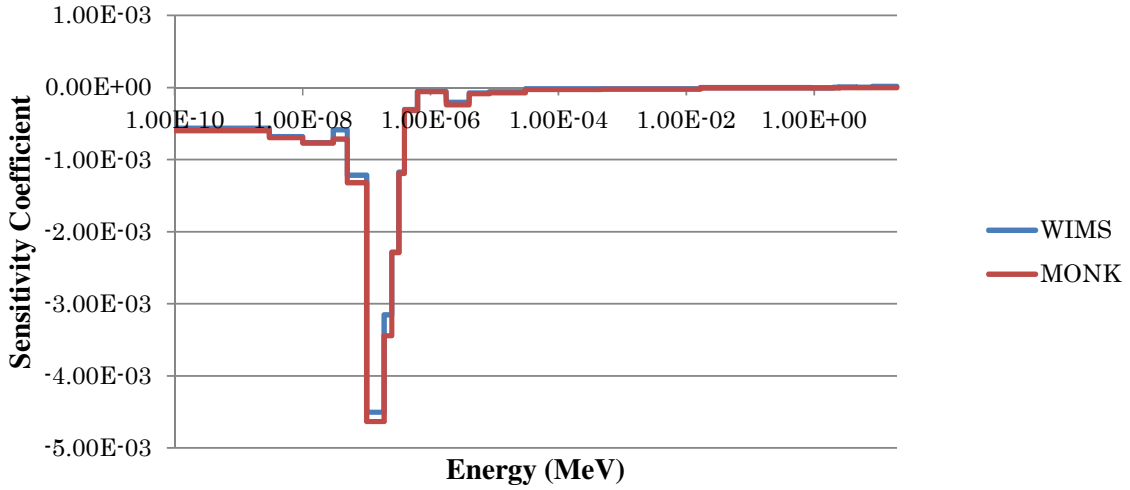

Figure 2. Comparison of MONK and WIMS sensitivity coefficients for U235 capture

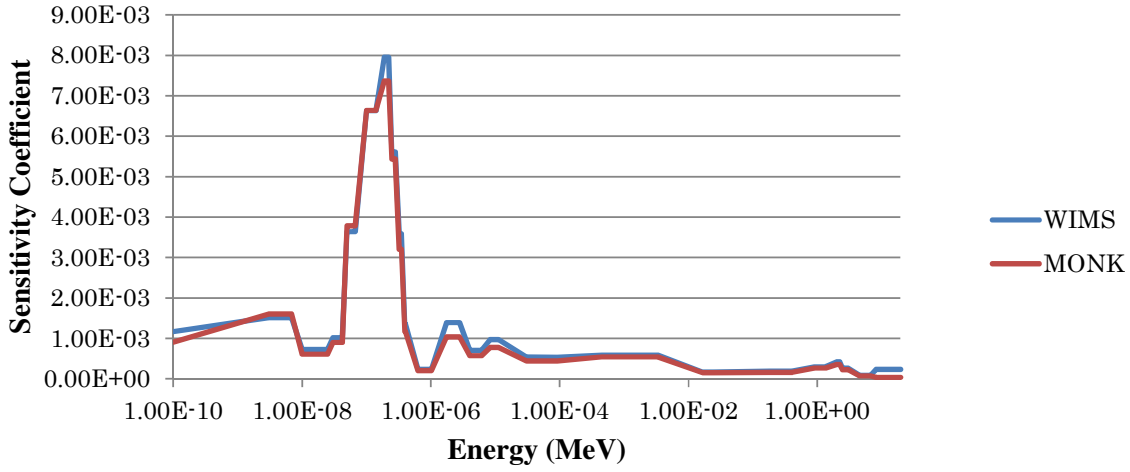

Figure 3. Comparison of MONK and WIMS sensitivity coefficients for U235 fission

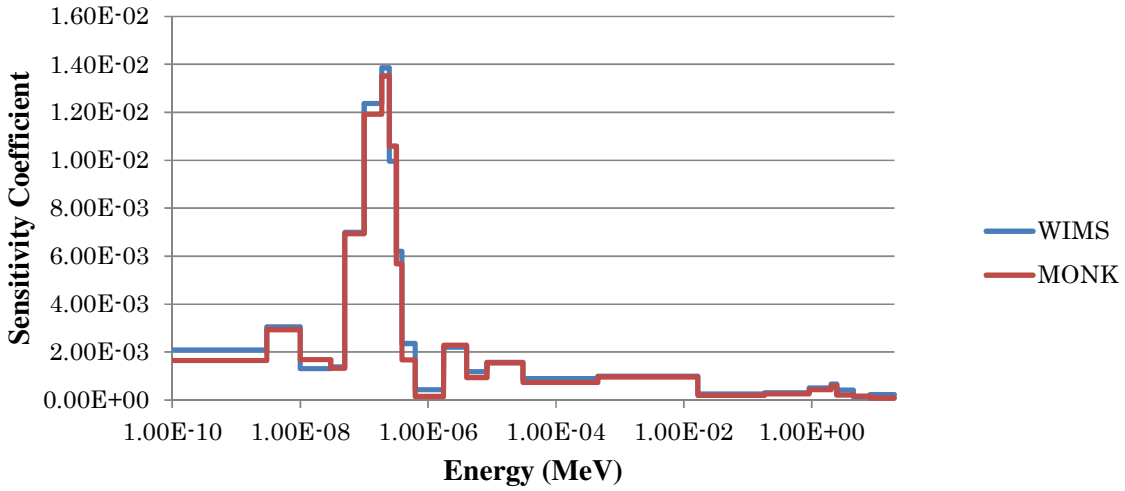

Figure 4. Comparison of MONK and WIMS sensitivity coefficients for U235 nubar

The sensitivity coefficients were combined with 44-group covariance data in order to estimate the uncertainties on k-infinity due to uncertainties on the microscopic cross-sections. It should be noted that, in WIMS, the cross-section perturbations are currently applied after resonance shielding. Therefore, the effects of perturbing cross-section data are not accounted for in the resonance shielding calculation. In future work, a methodology will be implemented to propagate the nuclear data uncertainties through the resonance shielding calculation. The uncertainty estimates are shown in Table 1; it is seen that there is close agreement between the MONK and WIMS estimates of k-infinity uncertainty due to U235 data.

Table 1. Comparison of % uncertainty values on k-infinity calculated by WIMS and MONK.

	WIMS	**MONK**
U235 nubar	0.28040	0.27740 ± 0.00175
U235 fission	0.14396	0.14430 ± 0.00032
U235 capture	0.14072	0.14120 ± 0.00014

4.2. Calculation of Contribution from Leakage for 1D model

When using the perturbation analysis method based on a MoC flux solution, the correct calculation of the leakage component of a k-effective change was confirmed using a 1D model. The 1D model consisted of 10 fuel regions, and a steel/water region as shown in Figure 5. In the unperturbed case, reflective boundary conditions were present at both ends of the model. In the perturbed case, a black boundary condition was utilized at the steel/water edge. In CACTUS, this is mimicked by specifying a thin region with a very-high absorption cross-section in all energy groups.

Figure 5. Test case geometry with fuel (red) and steel/water (blue) regions.

A reference value of k-effective was calculated directly for both perturbed and unperturbed systems. For this model, the difference between the perturbed and unperturbed values of k-effective gives the reactivity loss due to leakage in the perturbed system. The objective of this case is to demonstrate that this leakage term can be accurately calculated using the perturbation methodology.

The results of this test case are given in Table 2. As the macroscopic cross-sections of the perturbed and unperturbed systems are identical, the change in k-effective is entirely due to leakage. The total contribution of the leakage terms calculated using perturbation theory was confirmed to be an exact match to the absolute change in reactivity calculated directly, giving confidence in the methodology.

Table 2. Leakage effect on reactivity

k-effective (unperturbed system)	0.81470
k-effective (perturbed system) – directly calculated	0.78556
Reactivity difference – directly calculated	-2904pcm
Total reactivity difference calculated using perturbation methodology	-2904pcm

4.3. Cross-Section Perturbation for Slab Model

In this test case, a 3D slab model was created consisting of a mixture of enriched uranium fuel and structural material adjacent to relatively narrow regions of water (Figure 6). Reflective boundary conditions were applied on all external surfaces of the model. The hydrogen thermal scatter cross-section (in the energy range below 4 eV) was perturbed in all regions of the model. This causes a change in k-effective.

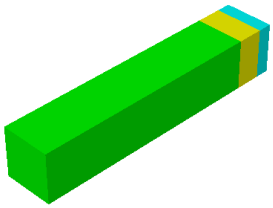

Figure 6. Slab Model consisting of fuel/water/structural material (green) and water (yellow & blue)

A calculation was performed using MONK (continuous-energy Monte Carlo) to estimate the k-effective change. Comparable calculations were made in WIMS using the CACTUS MoC solver and also a diffusion theory solver. The perturbation analysis tools in WIMS were used, in an exact rather than first-order form, to decompose the k-effective change into its scatter and leakage components.

Results from the analysis are shown in Table 3. It can be seen that the WIMS method of characteristics k-effective difference is in excellent agreement with MONK, while the diffusion theory solution differs somewhat.

From Table 3, it can be seen that diffusion theory and the method of characteristics are in excellent agreement in predicting the scatter term but differ significantly in their effect on the leakage term. This suggests that use of transport theory can be used to more accurately calculate the leakage term, which is supported by the excellent agreement between the WIMS and MONK solutions.

Table 3. Results from slab model analysis

	WIMS (Diffusion)	**WIMS (MoC)**	**MONK**
Unperturbed k-effective	1.78140	1.78114	1.77473 ± 0.00002
Perturbed k-effective	1.77967	1.78015	1.77570 ± 0.00002
k-effective difference (pcm)	-55	-31	-29 ± 3
of which due to leakage (pcm)	-82	-58	Not calculated
of which due to scatter (pcm)	28	27	Not calculated

5. CONCLUSIONS

This paper describes a new scheme to perform classical perturbation theory calculations that are based on transport theory flux solutions, through calculation of currents across all boundaries within a problem. This has been implemented in WIMS, and allows the response of a system to a perturbation to be analyzed by group, nuclide, region and energy group. The total uncertainty on k-infinity due to nuclear data uncertainty can be evaluated. Group-wise sensitivity coefficients are evaluated using the perturbation methodology which can then be combined with a nuclear data covariance library. It must be noted that further work is required to propagate the cross-section perturbations through the resonance shielding scheme in WIMS, which is ongoing. For the considered cases, excellent agreement was observed between WIMS and the Monte Carlo code MONK.

Compared to use of diffusion theory, using transport theory was shown to give a more accurate breakdown of the change in reactivity due to a perturbation using a simple test case with comparison to MONK. The perturbation methodology was used to demonstrate that this was due to a more accurate calculation of the leakage term using transport theory.

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