On Perturbation Components Correspondence Between Diffusion and Transport

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I. Transport equivalent Cross Sections

What shown in the following was inspired by work previously done by John Rowlands, to which this paper is dedicated.

In late 1970's John Rowlands pioneered the homogeneous/heterogeneous cross section equivalence based on reactivity conservation principle [1]. The methodology was implemented also in the ERANOS [2, 3] code system and allowed to calculate homogeneous equivalent cross sections that would take into account the spatial fine structure of sub-assemblies. It was successfully applied to fast reactor control rod calculations [4] in mid 1980's.

Similarly to Rowlands method the author proposed an algorithm to calculate transport equivalent cross sections to be used in diffusion calculations [5]. One has to keep in mind that in the 1980's the computing power was limited and three-dimensional transport calculations were prohibitively expensive and practically impossible.

The MONSTRE (Method to Obtain New Cross-Section Transport Equivalent) method defined cross sections to be used in a diffusion code that would reproduce the same reactivity variation (e.g. induced by control rod insertion) obtained using a transport code.

MONSTRE is based on a variational principle applied on the reactivity change between two cases, (reference and perturbed) calculated in transport and diffusion theory: To this purpose one can make use of the exact perturbation formulas in order to impose the equality between the two reactivity changes:

$$(\Sigma^P - \Sigma^R) < \varphi_P . \varphi_R^* >^{TR} - (\Sigma^x - \Sigma^R) < \varphi_x . \varphi_R^* >^{DIF} = 0 \qquad (1)$$

Where:
R: reference case index
P: perturbed case index
TR: transport theory calculation index
DIF: diffusion theory calculation index
$< \; >$: perturbation integrals over the perturbed region
Σ^x: transport equivalent cross section to be calculated
φ and φ^*: real and adjoint flux

If one requires Eq. (1) to be satisfied for each type of cross section the following equation is obtained:

$$\Sigma^x = (\Sigma^P - \Sigma^R) \frac{<\varphi^P . \varphi^R >^{TR}}{<\varphi^x . \varphi^R >^{DIF}} - \Sigma^R \qquad (2)$$

In Eq. (1) and (2), as in the case of homogeneous equivalent cross setions[1], an unknown flux φ_x is present. This flux is determined by an iterative procedure where the starting flux is the one calculated by diffusion theory. The iterative procedure is stopped when the reactivity variation calculated using the equivalent cross sections is equal to that of the transport calculation within the limit of a convergence criterion.

The equivalence between the different components, which corresponds to different cross sections, of the perturbation integrals in diffusion and transport have not been documented, and will be illustrated in next section. It will be seen that there is an interesting equivalence, regarding the leakage component that has implications on current investigations devoted to optimization of low sodium void reactivity coefficients fast reactors.

II. Diffusion and Transport Perturbation Components Equivalence

One can start from writing the transport equation in its multigroup form. One can neglect here the anisotropic scattering as it is not relevant to what it will be illustrated. For instance, one can adopt the transport approximation where the transport cross section replaces the total one.

The multigroup (first order formulation) transport equation can be written for group g as:

$$\nabla\Omega . \varphi_g(r,\Omega) + \Sigma_g^t . \varphi_g(r,\Omega) = \frac{\chi_g}{K_{eff}} \sum_{g'=1}^{NG} \nu\Sigma_g^f \varphi_g(r) + \sum_{g'=1}^{NG} \Sigma_{g' \to g}^{sc} \varphi_{g'}(r) \qquad (3)$$

where standard notation is used, NG is the total number of energy groups and Σ^t is the total cross section, Σ^f is the fission cross section Σ^{sc}, is the scattering one, and χ is the fission spectrum. In order to understand the different perturbation components one can notice that:

$$\Sigma^t = \Sigma^c + \Sigma^f + \Sigma^{sc} \qquad (4)$$

Where is Σ^c the capture cross section.

One can observe that in Eq. (3) the first term (the current gradient) does not contain any cross section, and all the angular dependence is on the left hand side of the equation.

Using the P_1 approximation for the anisotropy of the flux and Fick's law, one can write the corresponding diffusion equation:

$$\nabla D_g \nabla \varphi_g(r) + \Sigma_g^{Rem}. \varphi_g(r) = \frac{\chi_g}{K_{eff}} \sum_{g'=1}^{NG} \nu\Sigma_g^f \varphi_g(r) + \sum_{g'=1}^{NG,g' \neq g} \Sigma_{g' \to g}^{sc} \varphi_{g'}(r) \qquad (5)$$

Here the D_g is the diffusion coefficient and Σ^{Rem} is the removal cross section:

$$\Sigma_g^{Rem} = \Sigma_g^c + \Sigma_g^f + \sum_{g'=1}^{NG,g' \neq g} \Sigma_{g' \to g}^{sc} \qquad (6)$$

One can observe from inspection of Eq. (3) and (5) that:

- There is not anymore angular dependence in (5)
- The $\Sigma_{g \to g}^{sc}$ cross section does not appear in (5), but instead there is a term that uses the diffusion coefficient D_g.

In order to derive the perturbation formulas Eq. (3) and (5) are multiplied by the corresponding adjoint flux and integrated over the associated phase space. Two main types of perturbation integrals are used. One, $I_{gg'}^s$, is integrated only over the space variable:

$$I_{gg'}^s = \int \varphi_g(r). \varphi_{g'}^*(r) \, dr \qquad (7)$$

and the other, $I_{gg'}^a$, over both the space and angular variable

$$I_{gg'}^a = \int \varphi_g(r,\Omega). \varphi_{g'}^*(r,\Omega) \, dr d\Omega \qquad (8)$$

The (7) are used in the diffusion equation and in the transport equation for components that appear in the right hand side of Eq. (3). The (8) are used for components that appear on the left hand side of Eq. (4). The first term of Eq. (5), the leakage term I_g^L, makes use of the divergence theorem and requires an integration over the surface s instead of the volume of the perturbed region:

$$I_g^L = \int \nabla \varphi_g(s). \nabla \varphi_g^*(s) \, ds \qquad (9)$$

The first term, the production term, of both Eq. (4) and Eq. (5) requires two integrals for perturbation of the fission cross section and Nu-bar, I_g^{Fis}, and the fission spectrum, I_g^{Spec},:

$$I_g^{Fis} = \int \varphi_g(r). \sum_{g'=1}^{NG} \chi_{g'} \ \varphi_{g'}^*(r) \, dr \qquad (10)$$

$$I_g^{Spec} = \int \varphi_g^*(r). \sum_{g'=1}^{NG} \nu\Sigma_{g'}^f \ \varphi_{g'}(r)(r) \, dr \qquad (10)$$

Now one can compare one by one the perturbation component formulation in diffusion and transport. Table I shows this comparison for the different terms where the δ symbol implies the cross section variation between perturbed and reference configuration.

Table I. Comparison of Perturbation Component Formulation in Diffusion and Transport

Component	Diffusion	Transport
Capture	$\delta\Sigma_g^c I_{gg}^s$	$\delta\Sigma_g^c I_{gg}^a$
Fission	$\delta\Sigma_g^f (I_g^{Fis} - I_{gg}^s)$	$\delta\Sigma_g^f (I_g^{Fis} - I_{gg}^a)$
Scattering (g≠g')	$\delta\Sigma_{g \to g'}^{sc} (I_{gg'}^s - I_{gg}^s)$	$\delta\Sigma_{g \to g'}^{sc} (I_{gg'}^s - I_{gg}^a)$
Nu-bar.	$\delta\nu_g I_g^{Fis}$	$\delta\nu_g I_g^{Fis}$
Fiss. Spec.	$\delta\chi_g I_g^{Spec}$	$\delta\chi_g I_g^{Spec}$
Leakage	$\delta D_g I_g^L$	$\delta\Sigma_{g \to g}^{sc} (I_{gg}^s - I_{gg}^a)$

The Nu-bar and fission spectrum terms have the same formulation for both transport and diffusion. The first three terms have the same formulations except that the space integral of type (7) is replaced by an angular integral of type (8). This implies that in a case where the diffusion approximation is valid (P_1 approximation and Fick's law) the first 5 terms should give very comparable results.

What is left is the leakage term in diffusion and the $\delta\Sigma_{g \to g}^{sc}$ in transport. Again, if the diffusion approximation is valid these two terms should be now comparable, so that one has now an equivalent perturbation leakage term also in transport. It will be seen in next session that this is confirmed in practical cases. In the MONSTRE methodology this correspondence for the leakage term

allowed to successfully produce transport equivalent diffusion coefficients.

III. Practical Applications

Two cases will be considered for the practical applications, both of them fast reactors with sodium void as perturbation. The first one is the EFR (European Fast Reactor) system (model and characteristics are provided in reference [6]), which is a large size fast reactor with blankets, and sodium is voided in the core and blanket regions. One expects the diffusion approximation to work for this system and have very comparable results to those of a transport code. The second configuration is the ABR [7] (Advance Burner Reactor) in the oxide fuel with recycled minor actinides version that enhances the sodium void effect. Sodium is voided in the core zone and regions on top and bottom of the core. Because of the size f the ABR and the use of a radial reflector, instead of a blanket, significant differences are expected between diffusion and transport results. Calculations have been carried out using ERANOS, R-Z cylindrical models, and ENDF/B-VII.0 cross sections.

Table II shows the results obtained for the EFR.

Table II. Sodium Void Perturbation Components in Diffusion and Transport for EFR Reactor (pcm)

Component	Diffusion	Transport
Capture	380	378
Fission	101	101
Scattering (g≠g')	2647	2649
Leakage	-1165	-1163
Sum	1962	1964

Of course, because this is sodium void, there is no variation of Nu-Bar or fission spectrum. The variation on fission cross sections is due to the spectrum change between reference and voided configuration. As expected, results are very comparable (within 2 pcm) between diffusion and transport. The components are defined following the definitions provided in Table I; therefore, this confirms that the diffusion leakage perturbation

component corresponds to that of the group self scattering in transport.

Table III shows the results for the sodium void perturbation on the ABR reactor.

Table II. Sodium Void Perturbation Components in Diffusion and Transport for ABR Reactor (pcm)

Component	Diffusion	Transport
Capture	474	475
Fission	109	108
Scattering (g≠g')	3945	3905
Leakage	-3542	-2112
Sum	987	2376

Contrary to what observed in the EFR, the ABR total sodium void reactivity between diffusion and transport is quite different, confirming that for small/medium size reactors with radial reflectors transport theory is necessary. Looking at the components one can observe that almost the totality of the difference (except for a small difference of 40 pcm in the scattering component) is coming from the leakage one, where diffusion normally tend to overestimate the gradient effects.

IV. Conclusions

A correspondence between perturbation components in diffusion and transport theory has been established. In particular, the correspondence between the leakage perturbation component of the diffusion theory to that of the group self scattering in transport theory has been established. This has been confirmed by practical applications on sodium void reactivity calculations of fast reactors.

Why this is important for current investigations? Recently, there has been a renewed interest in designing fast reactors where the sodium void reactivity coefficient is minimized. In particular the ASTRID [8,9] reactor concept has been optimized with this goal in mind.

The correspondence on the leakage term that has been established here has a twofold implication for the design of this kind of reactors. First, this type of reactor

has a radial reflector; therefore, as shown before, the sodium void reactivity coefficient calculation requires the use of transport theory. The minimization of the sodium reactivity coefficient is normally done by increasing the leakage component that has a negative sign. The correspondence established in this paper allows to directly look at this component in transport theory.

The second implication is related to the uncertainty evaluation on sodium void reactivity. As it has shown before, the total sodium void reactivity effect is the result of a large compensation (opposite sign) between the scattering (called often spectral) component and the leakage one. Consequently, one has to evaluate separately the uncertainty on each separate component and then combine them statistically. If one wants to compute the cross section sensitivity coefficients of the two different components, the formulation established in this paper allows to achieve this goal by playing on the contribution to the sodium void reactivity coming from the group self scattering of the sodium cross section.

ACKNOWLEDGMENTS

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