Calculation of Coupling Coefficients of Coupled Reactors Theory Using the Generalized Perturbation Theory

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Recently, rigorous multi-point equations are derived using the region-wise importance functions to produce fission neutrons. Since the coupling coefficients used in these multi-point equations are calculated with the weight of these importance functions but not the adjoint function used in the conventional perturbation theory, errors due to the change of the flux is introduced in the coupling coefficients for a perturbed system if the unperturbed flux is used.

It is shown that using the generalized perturbation theory, the coupling coefficients using the unperturbed flux can be obtained taking into account the first order change of the flux due to the perturbation, and the same accuracy as the conventional perturbation theory in which the adjoint function is used can be obtained in the case of one-point reactor.

KEYWORDS: coupled reactors theory, coupling coefficients, coupling constants, generalized perturbation, importance function, adjoint function, perturbation theory, reactor kinetics, accuracy, errors

I. INTRODUCTION

Recently, rigorous multi-point kinetics equations are derived using importance functions to produce fission neutrons starting from the time dependent multi-group diffusion or transport equations(1)-(3). The unknown functions of these equations are the number of fission neutrons produced in each core or node. Since the coupling coefficients are obtained exactly independent of the strength of the coupling, we can use these equations as the nodal equations of the one-group form by dividing a core into appropriate nodes.

We can use these kinetics equations in a static form by introducing a criticality factor. In this case, the form of these nodal equations is similar as that used in the FLARE code which is a three-dimensional boiling water reactor simulator(4).

The coupling coefficients $k_{mn}$ in the multi-point equations, which express the number of neutrons produced in the node $m$ by a neutron born in the node $n$, corresponds to the product of the transport kernel $W_{nm}$ and the multiplication factor $k_m$ of the FLARE code, where $W_{nm}$ is the transport kernel which is the probability that a neutron born at node $n$ is absorbed at node $m$ and $k_m$ is the number of neutrons produced in node $m$. Then the coupling coefficients $k_{mn}$ can be regarded as the exact expression of the transport kernel $W_{nm}$ multiplied by $k_m$ used in the FLARE code, where only approximate expressions were given.

In order to calculate the coupling coefficients for the perturbed reactors exactly, we must use the flux for the perturbed reactors. If we calculate the coupling coefficients for the perturbed reactors using the unperturbed flux, approximate coupling coefficients are obtained which contains the error by the neglect of the change of the flux due to the perturbations.

If we use the generalized perturbation theory developed by Gandini et al.(5)(6), we can obtain integral quantities with the weight of the flux in which the change of flux due to the perturbation can be taken into account in the first order.

In the present work, using the generalized perturbation theory, a method is given to calculate the coupling coefficients using the unperturbed flux, but the change of the flux due to the perturbation is taken into account in the first order. These equations may be used as the nodal equations for the multi-group diffusion or transport equations.

II. THEORY OF COUPLED REACTORS

We consider here the problem in a frame of the diffusion equations for simplicity, and we assume that a multiplying system is described by the following multi-group diffusion equation:

$$L\phi_g(r) = \frac{1}{k}P\phi_g(r),$$

(1)

where the destruction and production operators $L$ and $P$ are defined by
respectively. Here, \( \phi_g(r) \) is the neutron flux of \( g \)-th group at the position \( r \), \( D_g \) the diffusion coefficient, \( \Sigma_{rg} \) the removal cross section, \( \Sigma_s(g \leftarrow g') \) the scattering cross section from the \( g' \)-th group to the \( g \)-th group, \( \chi_g \) the fission neutron spectrum, \( \nu \Sigma_{fg} \) the fission cross section multiplied by the number of fission neutrons and \( k \) the criticality factor.

The region-wise importance functions \( G_m(r, g) \) to produce fission neutrons are defined using the adjoint operator of the destruction operator \( L^\dagger \) by (1):

\[
L^\dagger G_m(r, g) = \nu \Sigma_{fg}(r) \delta_m(r), \quad m = 1, 2, \ldots,
\]

where \( \delta_m(r) \) takes 1 when \( r \) is in region \( V_m \), and 0 when \( r \) is outside of region \( V_m \), namely

\[
\delta_m(r) = \begin{cases} 
1, & r \in V_m \\
0, & r \notin V_m.
\end{cases}
\]

We use the same boundary condition for the flux of Eq. (1) and the importance function of Eq. (3) that they vanish at the outer most boundary of the reactor. This importance function \( G_m(r, g) \) has the physical meaning of the number of fission neutrons produced in a region \( V_m \) by a neutron born at position \( r \) with an energy group \( g \).

Multiplying Eq. (1) by the importance function of Eq. (3), integrating it over whole reactor \( V \) and summing it up over all energy groups, we obtain the multi-point equations for fission sources

\[
S_m = \frac{1}{k} \sum_n k_{mn} S_n,
\]

where \( S_m \) is the fission source in region \( V_m \) defined by

\[
S_m = \int_{V_m} s(r) dr,
\]

and \( k_{mn} \) are the coupling coefficient given by

\[
k_{mn} = \frac{\int_{V_m} dr \Sigma_g G_m(r, g) \chi_g s(r)}{\int_{V_m} dr s(r)}.
\]

1. Perturbed System by the Coupled Reactors Theory

We assume that a perturbation is introduced to a reactor, and operators \( L \) and \( P \) and hence the neutron flux change slightly, namely

\[
L \rightarrow \bar{L} = L + \delta L, \\
P \rightarrow \bar{P} = P + \delta P,
\]

\[
\phi \rightarrow \bar{\phi} = \phi + \delta \phi.
\]

The notation \( - \) is used to denote the quantity for perturbed system. The diffusion equation for the perturbed system is written as

\[
\bar{L} \bar{\phi}_g(r) = \frac{1}{k} \bar{P} \bar{\phi}_g(r),
\]

where \( \bar{k} \) is the criticality factor for the perturbed system. The multi-point equations for the perturbed system can be derived similarly as (3)

\[
\bar{S}_m = \sum_n \left( \frac{1}{k} \bar{k}_{mn} + \Delta k_{mn}^{F} \delta_m - \Delta k_{mn}^{A} \right) \bar{S}_n,
\]

where \( \Delta k_{mn}^{F} \) and \( \Delta k_{mn}^{A} \) are the change of the coupling coefficients due to the explicit change of the operator by the perturbation given by

\[
\Delta k_{mn}^{F} = \int_{V_m} \frac{dr \delta F \bar{\phi}_g(r)}{\int_{V_m} dr \bar{s}(r)},
\]

and

\[
\Delta k_{mn}^{A} = \int_{V_m} \frac{dr \Sigma_g G_m(r, g) \delta F \bar{\phi}_g(r)}{\int_{V_m} dr \bar{s}(r)},
\]

respectively. The coupling coefficients \( \bar{k}_{mn} \) in Eq. (10), which are given by Eq. (7) with the perturbed flux, change due to the perturbation in the flux. If we calculate them using the unperturbed flux by ignoring the change of the flux \( \delta \phi \), the coupling coefficients will have the error due to the neglect of the first order change of the flux. In Eqs. (11) and (12), the unperturbed flux can be used, since the error by its use is the second order.

2. Application of the Generalized Perturbation Theory

This first order error due to the use of the unperturbed flux in calculating \( \bar{k}_{mn} \) can be removed by use of the generalized perturbation theory developed by Gandini et al. (5)(6).

We rewrite the coupling coefficient as

\[
\bar{k}_{mn} = \int_{V_m} \frac{dr \Sigma_g G_m(r, g') \chi_g \Sigma_g \nu \bar{\Sigma}_{f_g}(r) \bar{\phi}_g(r)}{\int_{V_m} dr \Sigma_g \nu \bar{\Sigma}_{f_g}(r) \bar{f}_g(r)}
\]

\[
= \int_{V_m} \frac{dr \Sigma_g \tilde{\Sigma}_{1g}(r) \bar{\phi}_g(r)}{\int_{V_m} dr \Sigma_g \tilde{\Sigma}_{2g}(r) \bar{\phi}_g(r)},
\]

where the fictitious cross sections \( \tilde{\Sigma}_{1g}(r) \) and \( \tilde{\Sigma}_{2g}(r) \) are defined by

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\[ \bar{\Sigma}_{1g}(r) = \sum_{g'} G_m(r, g') \chi_{g'} \nu \Sigma_{fg}(r) \delta_n(r), \]  
\[ \bar{\Sigma}_{2g}(r) = \nu \Sigma_{fg}(r) \delta_n(r), \]
respectively.

We write the change of the fictitious cross section due to the perturbation as \[ S_1 = S_1 + dS_1, \quad S_2 = S_2 + dS_2. \] The perturbed coupling coefficient \( k_{mn} \) due to the perturbation can be written neglecting the second order term of the perturbation as

\[ \hat{k}_{mn} = \frac{\left( \Sigma_1 + \delta \Sigma_1 \right) (\phi + \delta \phi)}{\left( \Sigma_2 + \delta \Sigma_2 \right) (\phi + \delta \phi)} \]
\[ = \frac{\left( \Sigma_1 \phi \right) + \left( \Sigma_1 \delta \phi \right) + \left( \delta \Sigma_1 \phi \right)}{\left( \Sigma_2 \phi \right) + \left( \Sigma_2 \delta \phi \right) + \left( \delta \Sigma_2 \phi \right)} \]
\[ = \frac{\left( \Sigma_1 \phi \right)}{\left( \Sigma_2 \phi \right)} \left( 1 + \frac{\left( \Sigma_1 \delta \phi \right)}{\left( \Sigma_1 \phi \right)} + \frac{\left( \delta \Sigma_1 \phi \right)}{\left( \Sigma_1 \phi \right)} \right) \]
\[ - \frac{\left( \Sigma_2 \delta \phi \right)}{\left( \Sigma_2 \phi \right)} - \frac{\left( \delta \Sigma_2 \phi \right)}{\left( \Sigma_2 \phi \right)}, \]
where \( \left( \Sigma_1 \phi \right) = \int_V dr \Sigma_{1g}(r) \phi_g(r). \)

We use the generalized perturbation theory to calculate the first order terms of the change of the flux, \( \delta \Sigma_1 \delta \phi \) and \( \delta \Sigma_2 \delta \phi \). Using the operator \( H, H = L - \frac{1}{k} P \), we write Eq. (1) as

\[ H \phi = \left( L - \frac{1}{k} P \right) \phi = 0. \]  
After the introduction of the perturbation, the operator \( H \) changes to \( H + \delta H \), and Eq. (17) changes to the equation;

\[ (H + \delta H)(\phi + \delta \phi) = 0. \]  
Neglecting the second order terms due to the perturbation, Eq. (18) becomes

\[ H \delta \phi + \delta H \phi = 0. \]  
The change of the operator \( H \) due to the perturbation can be written as

\[ \delta H = H + \delta H - H \]
\[ = L + \delta L - \frac{1}{k} (P + \delta P) - \left( L - \frac{1}{k} P \right) \]
\[ = \delta L - \frac{1}{k} \delta P + \rho P, \]  
where the reactivity \( \rho \) is defined by

\[ \rho = \frac{1}{k} - \frac{1}{k}. \]  
Using the adjoint operator \( H^\dagger \) of the operator \( H \) and the source term \( q^\dagger \) defined by

\[ q^\dagger = \frac{\Sigma_1}{(\Sigma_1 \phi)} - \frac{\Sigma_2}{(\Sigma_2 \phi)}, \]
we consider an adjoint solution \( \phi^\dagger_q \) of the following equation;

\[ H^\dagger \phi^\dagger_q = q^\dagger. \]  
For the existence of a solution for Eq. (23) with the source term \( q^\dagger \), the source term \( q^\dagger \) must satisfy the following condition;

\[ \langle \phi^\dagger_q r \rangle = 0, \]  
which means that the source term should not contain the fundamental mode of the operator \( H \), and this condition is satisfied by the source term of Eq. (22).

Multiplying Eq. (19) by \( \phi^\dagger_q \), we obtain

\[ \langle \phi^\dagger_q H \delta \phi + \phi^\dagger_q \delta H \phi \rangle = 0, \]
\[ \langle \delta \phi H^\dagger \phi^\dagger_q \rangle = -\langle \phi^\dagger_q \delta H \phi \rangle. \]  
Using Eq. (23), we obtain

\[ \langle \delta \phi q^\dagger \rangle = -\langle \phi^\dagger_q \delta H \phi \rangle. \]  
Substituting Eq. (22) into Eq. (26), we obtain

\[ \langle \delta \phi \Sigma_1 \rangle - \langle \delta \phi \Sigma_2 \rangle = -\langle \phi^\dagger_q \delta H \phi \rangle. \]  
Using Eqs. (20) and (27), Eq. (16) becomes

\[ \hat{k}_{mn} = \frac{\Sigma_1 \phi}{\Sigma_2 \phi} \left( 1 + \frac{\delta \Sigma_1 \phi}{\Sigma_1 \phi} + \frac{\delta \Sigma_2 \phi}{\Sigma_2 \phi} \right) \]
\[ - \frac{\delta \Sigma_2 \phi}{\Sigma_2 \phi} - \frac{\delta \Sigma_2 \phi}{\Sigma_2 \phi}, \]
where \( \langle \Sigma_1 \phi \rangle = \int_V dr \Sigma_{1g}(r) \phi_g(r). \)

\[ H^\dagger \phi^\dagger_q = \rho \phi^\dagger_q, \]  
where \( \alpha \) is a constant and \( \phi^\dagger_q \) is a solution of the homogeneous equation;

\[ H^\dagger \phi^\dagger_q = 0, \]  
which has a non-zero solution as seen in Eq. (17). The \( \phi^\dagger_q \) is a particular solution of inhomogeneous equation of Eq. (23) with the source term \( q^\dagger \). In order to determine the constant \( \alpha \) uniquely, we must use an additional condition. If we use the condition

\[ \langle \phi^\dagger_q P \phi \rangle = 0, \]
the last term of Eq. (28) vanishes, which is convenient, since \( \rho \) is an unknown quantity*. Using this condition, we can calculate the coupling coefficient of Eq. (28) in which the first order change of the flux is taken into account using the unperturbed flux.

**III. Simple Example**

In order to investigate the accuracy of the coupling coefficient derived in the preceding chapter, let us con-

*The explanation for the last term of Eq. (10.219) in page 675 of Ref. 7 is wrong. It should be replaced by the above.
sider a simple problem with one point model in order to compare the accuracy with the conventional perturbation theory.

We consider a slab reactor of a thickness $a$ with the one group diffusion equation given by

$$
( -D \frac{d^2}{dx^2} + \Sigma_a ) \phi(x) = \frac{1}{k} k_{\infty} \Sigma_a \phi(x),
$$

(32)

where $\Sigma_a$ is the absorption cross section and $k_{\infty}$ the infinite multiplication factor.

Choosing the origin of the coordinate at the center of the slab reactor, the flux and the criticality factor are given by

$$
L^2 = \frac{D}{\Sigma_a}, \quad B = \frac{\pi}{a}.
$$

(33)

We consider a simple perturbation, where the absorption cross section $\delta \Sigma_a = \Delta \Sigma_a T \delta(x - \xi)$, $T$ being the thickness of the absorber, is added at $\xi$, namely, we consider the following equation for perturbed system;

$$
( -D \frac{d^2}{dx^2} + \Sigma_a + \Delta \Sigma_a T \delta(x - \xi) ) \phi(x) = \frac{1}{k} k_{\infty} \Sigma_a \phi(x).
$$

(34)

1. Exact Solution

The exact solution of Eq. (34) can be easily obtained as follows. Integrating Eq. (34) around the singular point at $x = \xi$, we obtain the condition

$$
- D \frac{d\phi(x)}{dx} \bigg|_{x = \xi} = - \Delta \Sigma_a T \phi(\xi),
$$

(35)

which must be satisfied by the flux.

The solution of Eq. (34) is given by

$$
\phi^- (x) = A \sin \tilde{B} \left( \frac{a}{2} + x \right), \quad \text{for} \quad x \leq \xi,
$$

$$
\tilde{B} = \frac{1}{L} \sqrt{\frac{k_{\infty}}{k} - 1},
$$

(36)

and

$$
\phi^+ (x) = C \sin \tilde{B} \left( \frac{a}{2} - x \right), \quad \text{for} \quad x \geq \xi,
$$

$$
\tilde{B} = \frac{1}{L} \sqrt{\frac{k_{\infty}}{k} - 1},
$$

where $A$ and $C$ are constants, which can be determined by applying the condition of Eq. (35) and the continuity of the flux at $x = \xi$, namely

$$
D \tilde{B} \cos \left[ \tilde{B} \left( \frac{a}{2} + \xi \right) \right] A + D \tilde{B} \cos \left[ \tilde{B} \left( \frac{a}{2} - \xi \right) \right] C
$$

$$
- \Delta \Sigma_a T \sin \left[ \tilde{B} \left( \frac{a}{2} + \xi \right) \right] A,
$$

(37)

and

$$
\sin \left[ \tilde{B} \left( \frac{a}{2} + \xi \right) \right] A - \sin \left[ \tilde{B} \left( \frac{a}{2} - \xi \right) \right] C = 0.
$$

(38)

The criticality factor $\tilde{k}$ can be obtained numerically such that the determinant of the coefficients matrix of Eqs. (37) and (38) vanishes.

2. Criticality Factor by the Perturbation Method

Since Eq. (32) is self-adjoint, the adjoint function $\phi^*(x)$ for Eq. (32) is the same as the solution of Eq. (32), namely, $\phi^*(x) = \phi(x)$. Then the reactivity due to the conventional perturbation theory is given using the direct and adjoint fluxes for unperturbed system by

$$
\rho = \frac{1}{k} \frac{1}{\tilde{k}} = \frac{\langle \phi^* \delta \Sigma_a T \phi \rangle}{\langle \phi^* \kappa \Sigma_a \phi \rangle} = \frac{\Delta \Sigma_a T \cos \beta}{k_{\infty} \Sigma_a a/2},
$$

(39)

from which we can obtain the criticality factor $\tilde{k}$ for the perturbed system.

3. Criticality Factor by the Coupled Reactors Theory

From Eq. (10), we obtain the criticality factor for the perturbed system as

$$
\frac{1}{k} = \frac{1}{\tilde{k}} (1 + \Delta k_{11}^d).
$$

(40)

We calculate the approximate coupling coefficients using the unperturbed flux. In the case of one region, the importance function of Eq. (3) can be obtained as

$$
G(x) = k_{\infty} \left( 1 - \frac{\cosh \kappa x}{\cosh \frac{\kappa a}{2}} \right), \quad -\frac{a}{2} \leq x \leq \frac{a}{2},
$$

where $\kappa = \frac{1}{L}$.

(41)

Using this importance function, Eqs. (7) and (12) with the unperturbed flux, we obtain

$$
\tilde{k}_{11} = \int_{-a/2}^{a/2} G(x) \tilde{F} \phi(x) = \frac{k_{\infty}}{1 + L^2 B^2} = k,
$$

(42)

$$
\Delta k_{11}^d = \frac{\int_{-a/2}^{a/2} G(x) \delta A \phi(x)}{\int_{-a/2}^{a/2} \tilde{F} \phi(x)} = \frac{G(\xi) \Delta \Sigma_a T B \cos \beta \xi}{2k_{\infty} \Sigma_a}.
$$

(43)

Using these coupling coefficients, the criticality factor $\tilde{k}$ is obtained from Eq. (40).

4. Coupling Coefficient by the Generalized Perturbation Method

From Eqs. (14) and (15), we obtain the fictitious cross sections as

$$
\Sigma_1 = k_{\infty} \Sigma_a G(x), \quad \Sigma_2 = k_{\infty} \Sigma_a,
$$

(44)

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and Eq. (23) becomes

\[
\left(-D \frac{d^2}{dx^2} + \Sigma_a \right) \phi^i_0(x) - \frac{1}{k} \kappa_\infty \Sigma_a \phi^0_q(x) = q^i(x),
\]

with the source term of Eq. (22) given by

\[
q^i(x) = \frac{B(B^2 + \kappa^2)}{2\kappa^2} \left(1 - \frac{\cosh \kappa x}{\cosh \frac{\kappa a}{2}}\right) - \frac{B}{2},
\]

where \(\phi(x) = \cos Bx\) is used.

Using the Green’s function for Eq. (45) given by

\[
G(x, x') = \frac{1}{DB \sin Ba} \sin B \left(\frac{a}{2} - x\right) \sin B \left(\frac{a}{2} + x'\right),
\]

where \(x' \leq x\),

\[
= \frac{1}{DB \sin Ba} \sin B \left(\frac{a}{2} + x\right) \sin B \left(\frac{a}{2} - x'\right),
\]

\(x \leq x'\),

the solution of Eq. (45) with the source term of Eq. (46) can be obtained as

\[
\phi^i_0(x) = \int_{-a/2}^{a/2} G(x, x') q^i(x') dx'.
\]

The constant \(\alpha\) is determined such that the solution of Eq. (48) should satisfy Eq. (31), and we obtain the solution,

\[
\phi^i_0(x) = \frac{2}{aD(B^2 + \kappa^2)} \cos Bx - \frac{B}{2\Sigma_a k_\infty} G(x).
\]

Using Eq. (28) and \(\phi(x) = \cos Bx\), we obtain

\[
\bar{k}_{11} = \langle \Sigma_1 \phi \rangle \langle \Sigma_2 \phi \rangle (1 - \langle \phi^i_0(\delta L \phi) \rangle)
\]

\[
= \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle} (1 - \phi^i_0(\xi) \Delta \Sigma_a T \cos B\xi).
\]

Using Eqs. (42) and (44), we have

\[
\frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle} = k_{11} = \frac{k_\infty}{1 + L^2 B^2} = k.
\]

Then \(\bar{k}_{11}\) of Eq. (50) becomes

\[
\bar{k}_{11} = k(1 - \phi^i_0(\xi) \Delta \Sigma_a T \cos B\xi).
\]

Using Eqs. (43) and (52) in Eq. (40) and retaining the first order terms, we obtain the criticality factor for the perturbed system by using the generalized perturbation method as

\[
\frac{1}{k} = -\frac{1}{k} \left(1 + \frac{G(\xi) \Delta \Sigma_a T \cos B\xi}{2k_\infty \Sigma_a / B}\right)
\]

\[
= \frac{1}{k} \left(1 + \frac{BG(\xi) \Delta \Sigma_a T \cos B\xi}{2k_\infty \Sigma_a / B}\right),
\]

We can see that this criticality factor is just the same as Eq. (39) obtained by the conventional perturbation theory as expected.

Numerical results for the criticality factor for perturbations \(\Delta \Sigma_a T = 0 \sim 0.02\) are shown in Fig. 1, where the constants \(D = 1\ \text{cm}, \Sigma_a = 0.1\ \text{cm}^{-1}, k_\infty = 1.00987, a = 100\ \text{cm}\) and \(\xi = a/4\) are used. The criticality factor without the perturbation is 1.

Since the size of the reactor \(a = 100\ \text{cm}\) is much larger than the diffusion length \(L = \sqrt{10}\ \text{cm} = 3.16\ \text{cm}\), the flux changes largely by the flux tilt even by the very small perturbation as shown in Fig. 2 for the case of \(\Delta \Sigma_a T = 0.02\).

In the Fig. 1 are shown the exact criticality factors calculated by Eqs. (37) and (38), those of Eq. (39) by the conventional perturbation theory, \(\bar{k}\) of Eq. (40) by the coupled reactors theory, and those of Eq. (53) by the

![Fig. 1 Criticality factor \(\bar{k}\) as a function of the perturbation \(\Delta \Sigma_a T\)](image1)

![Fig. 2 Flux distributions for unperturbed and perturbed system of \(\Delta \Sigma_a T = 0.02\)](image2)
generalized perturbation theory. There is no difference on the Figure between $k$ by the conventional perturbation theory and by the generalized perturbation method as expected.

IV. CONCLUSION

A method to calculate the coupling coefficients for the perturbed system has been derived using the generalized perturbation method. It was shown that this method could take into account the first order change of the flux due to the perturbation and had the same accuracy as the conventional perturbation theory. Although in the present work, a simple problem was solved analytically, there is no difficulty to calculate the importance functions, the adjoint function $\phi^1_s(r)$ and the coupling coefficients for practical problems by solving the multi-group diffusion or transport equations numerically.

—REFERENCES—