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Numerical Calculation of λ-Mode of the Diffusion Equation

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수치해법을 이용한 중성자 확산방정식의 λ-Mode 계산

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Abstract

A successive iteration method to calculate the λ-modes of the diffusion equation was developed. The 2-group, 3-dimensional computer code MOGEN was developed to implement this method. The accuracy of the method was demonstrated using 2-dimensional bare homogeneous rectangular reactor. The numerical solution shows good agreement with the analytic solution in terms of eigenvalue and eigenfunction. As for the standard CANDU-600 reactor, the 2-dimensional modes were generated and these represent the conventional mode characteristics well. Finally, application of the λ-mode in reactor engineering problems is described briefly.

요 약

중성자 확산 방정식의 λ-mode를 구하는 반복 계산법을 정립하였고, 이 방법을 이용한 2군, 3차원 전산 코드 MOGEN을 개발하였다. 2차원 직각형 균질 원자로에 대해 계산을 수행하여, 생산된 고유치와 고유함수가 해석해에 잘 일치함을 보여 코드의 정확도를 검증하였다. 실제 CANDU형 표준 원자로의 2차원 mode를 생산하였고, 이는 기존의 mode 특성을 정확히 나타내었다. 마지막으로, λ-mode의 응용분야에 대하여 간략히 설명하였다.

1. Introduction

In many engineering problems, practical solutions can be obtained by replacing the rigorous equations that govern the system by a set of approximate equations with reduced number of independent variables, which is more tractable to solve.

The higher harmonics of the steady state diffusion equation (also called λ-modes) have been used in the modal expansion technique. A distinctive feature of this technique is that fewer terms in expansion are required to describe the perturbed flux distributions, since the λ-modes are more representative of physical characteri-

stics of the reactor system than any other functions. [3]

Although their usefulness has been appreciated in many references, their practial applications have been limited due to the requirement that they be calculated numerically and due to the lack of appropriate computer codes. One method to calculate the λ-modes has been described in reference [4], after which the present study has been patterned and the 2-group, 3-dimensional λ-mode generation code MOGEN was developed. (*)

2. Theory

2.1. Successive Iteration Method

We define λ-modes as the eigenfunctions which satisfy the 2-group static neutron diffusion equations;

$$-\nabla\cdot D_1(r)\nabla\varphi_{n_1}(r)+[\Sigma_{a_1}(r)+\Sigma_R(r)]\varphi_{n_1}(r)=\frac{1}{\lambda^n}[\nu\Sigma_{f_1}(r)\varphi_{n_1}(r)+\nu\Sigma_{f_2}(r)\varphi_{n_2}(r)] \quad -\nabla\cdot D_2(r)\nabla\varphi_{n_2}(r)+\Sigma_{a_2}(r)\varphi_{n_2}(r)=\Sigma_R(r)\varphi_{n_1}(r) \tag{1}$$

or in matrix form;

$$R\phi_n=\frac{1}{\lambda_n}M\phi_n \quad (n=1,2,\cdots\cdots) \tag{2}$$

In this expression, R and M are regarded as the destruction and production matrices respectively;

$$R=\begin{bmatrix} -\nabla\cdot D_1\nabla+\Sigma_{a_1}+\Sigma_R & 0 \\ -\Sigma_R & -\nabla\cdot D_2\nabla+\Sigma_{a_2} \end{bmatrix}$$

$$M=\begin{bmatrix} \nu\Sigma_{f_1} & \nu\Sigma_{f_2} \\ 0 & 0 \end{bmatrix}$$

where,

D_1 =fast diffusion coefficient
D_2 =thermal diffusion coefficient
Σ_{a_1} =fast absorption c.x.
Σ_{a_2} =thermal absorption c.x.
$\nu\Sigma_{f_1}$ =fast fission production c.x.
$\nu\Sigma_{f_2}$ =themal fission production c.x.
Σ_R =removal c.x.

Note that the fundamental mode is the eigenfunction corresponding to the largest eigenvalve λ_1, and other higher modes are the eigenfunctions corresponding to the next lower eigenvalues.

The purpose of this study is to find the eigenvalues λ_n and eigenfunctions ϕ_n of the matrix eq. (2).

The usual iterative procedure, where the fundamental mode is desired, starts with some guessed distribution $\phi_1^{(0)}$.

This can be expressed by the linear combination of the eigenfunctions of eq. (2) which make a complete set, i.e;

$$\phi_1^{(0)}=\sum_{i=1}^{\infty}a_i\varphi_i \tag{3}$$

The intermediate solution after l-th iteration can be written;

$$\phi_1^{(l)}=R^{-1}M\phi_1^{(l-1)}=\cdots=(R^{-1}M)^l\,\phi_1^{(0)} \tag{4}$$

By eq.(3);

$$\phi_1^{(l)}=(R^{-1}M)^l\sum_{i=1}^{\infty}a_i\varphi_i=\sum_{i=1}^{\infty}a_i(R^{-1}M)^l\varphi_i=\sum_{i=1}^{\infty}a_i\lambda_i^l\varphi_i=a_1\lambda_1^l\varphi_1+\sum_{i=2}^{\infty}a_i\lambda_i^l\varphi_i=\lambda_1^l[a_1\varphi_1+\sum_{i=2}^{\infty}a_i\left(\frac{\lambda_i}{\lambda_1}\right)^l\varphi_i] \tag{5}$$

Assume that the eigenvalues satisfy;

$$|\lambda_1|>|\lambda_2|>\cdots>|\lambda_n| \tag{6}$$

For sufficient large number of iteration L;

$$\phi_1^{(L)}\cong a_1\lambda_1^L\varphi_1\propto\varphi_1 \tag{7}$$

As a result, one obtains the eigenfunction φ_1

(*) The MOGEN was developed for 3-dimensional model, but in this study the calculation is performed to 2-dimensional problem for the convenience of result drawing and to compare with analytic one easily.

corresponding to the largest eigenvalue λ_1 which is called 'fundamental mode'. Due to the existence of a predominant mode, after some iterations, convergence on the higher harmonics can be realized by subtracting out those modes which are already known from the unconverged mode.

For the second mode, the calculation starts with some initial mode $\phi_2^{(0)}$ as in the previous case, i.e;

$$\phi_2^{(0)}=\sum_{i=1}^{\infty}a_i\varphi_i \tag{8}$$

Multiplying both sides of eq.(8) by φ_1^* M, where φ_1^* is the first eigenfunction of the adjoint to eq.(2) and M is the production matrix of eq.(2).

Integrating over the reactor volume, one obtains;

$$\int_R \varphi_1^* M\phi_2^{(0)}\ d^3r=\sum_{i=1}^{\infty}a_i\int_R \varphi_1^* M\varphi_i d^3r \tag{9}$$

On applying the well known bi-orthogonality condition;

$$\int_R \varphi_j^* M\varphi_i\ d^3r=0,\ \text{when } j\neq i \tag{10}$$

the amplitude of the fundamental mode component in initial mode is;

$$a_1^{(0)}=\frac{\int_R \varphi_1^* M\phi\phi_2^{(0)}d^3r}{\int_R \varphi_1^* M\varphi_1 d^3r} \tag{11}$$

Upon obtaining $a_1^{(0)}$ using eq.(11) and having already calculated φ_1 previously, the intermediate second mode is now expressed as;

$$\phi_2^{(1)}=\phi_2^{(0)}-a_1^{(0)}\varphi_1 \tag{12}$$

With this corrected $\phi_2^{(1)}$, next iteration is initiated involving the same procedure described above. During each iteration, the intermediate second mode ϕ_2 is updated by eq.(12), with a_1 that is updated by eq. (11).

After m-th iteration where m is sufficient number of iteration to remove fundamental component, one obtains;

$$\phi_2^{(m)}=\phi_2^{(m-1)}-a_1^{(m-1)}\varphi_1$$

$$\cong\sum_{i=2}^{\infty}a_i\varphi_i \tag{13}$$

For additive l iteration;

$$\begin{aligned}\phi_2^{(m+l)}&=R^{-1}M\phi_2^{(m+l-1)}\\&=\cdots\\&=(R^{-1}M)^l\phi_2^{(m)}\\&\cong(R^{-1}M)^l\sum_{i=2}^{\infty}a_i\varphi_i\\&=\sum_{i=2}^{\infty}a_i(R^{-1}M)^l\varphi_i\\&=\sum_{i=2}^{\infty}a_i\lambda_i^l\varphi_i\\&=a_2\lambda_2^l\varphi_2+\sum_{i=3}^{\infty}a_i\lambda_i^l\varphi_i\\&=\lambda_2^l\left[a_2\varphi_2+\sum_{i=3}^{\infty}a_i\left(\frac{\lambda_i}{\lambda_2}\right)^l\varphi_i\right.\end{aligned} \tag{14}$$

For sufficient large number of iteration L;

$$\begin{aligned}\phi_2^{(L)}&\cong a_2\lambda_2^L\varphi_2\\&\propto\varphi_2\end{aligned} \tag{15}$$

The solution should converge on the second mode φ_2 i.e. the harmonics corresponding to the next largest eigenvalue λ_2.

In general, for the $n+1$ the mode;

$$\phi_{n+1}^{(l)}=\phi_{n+1}^{(l-1)}-\sum_{i=1}^{n}a_i^{(l-1)}\varphi_i \tag{16}$$

where,

$$a_i^{(l-1)}=\frac{\int_R \varphi_i^* M\phi_{n+1}^{(l-1)}d^3r}{\int_R \varphi_i^* M\varphi_i d^3r} \tag{17}$$

In this manner, all harmonics can be calculated in principle.

2.2. Self-Adjoint Property of the 1-group Flux

To calculate the amplitude of the previous mode, one must evaluate the adjoint mode corresponding to the direct mode. By similar procedure described in the previous section, adjoint mode can be generated from the adjoint equations of eq.(1) using the precalculated direct modes as weight functions in calculating the amplitudes. But this requires the same amount of computing effort as to calculate the direct modes.

To avoid this extra work, an approximate method is presented.

Following the suggestion of reference [4], the self-adjoint property of 1-group flux was utilized, and it was again found that the calculated λ-modes were indistinguishable from those obtained with the exact bi-orthogonality property stated in eq.(10).

Consequently, the adjoint calculations was removed and the pseudo-one-group flux;

$$\varphi_n^p=\varphi_{n_1}+\varphi_{n_2} \tag{18}$$

in now used in conjunction with the orthogonality property;

$$\int_R \varphi_j^p M\varphi_i \, d^3r=0, \quad \text{when } j\neq i \tag{19}$$

to obtain residual mode amplitudes in the unconverged mode.

3. Sample Problems

The calculational method described in the previous sections was tested for 2-dimensional bare homogeneous rectangular reactor having zero flux boundary condition. Reactor geometry and nuclear data are given Figure 1 and Table 1 respectively.

The problem was solved both analytically and numerically to compare its accuracy.

Table 1. Nuclear Data

group	D (cm)	Σ_a(cm^{-1})	$\nu\Sigma_f$(cm^{-1})	Σ_R(cm^{-1})
1	1.5	0.01	0.007	0.01
2	0.5	0.15	0.4	0.0

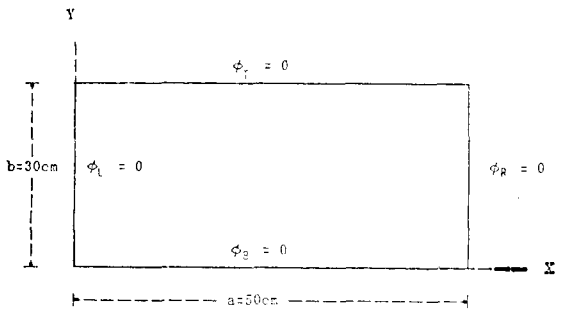


Fig. 1. Reactor Geometry

The 2-group diffusion equations for this example are as follows;

$$-D_1\left(\frac{\partial^2\phi_1}{\partial x^2}+\frac{\partial^2\phi_1}{\partial y^2}\right)+(\Sigma_{a_1}+\Sigma_R)\phi_1$$
$$=\frac{1}{\lambda}(\nu\Sigma_{f_1}\phi_1+\nu\Sigma_{f_2}\phi_2)$$
$$-D_2\left(\frac{\partial^2\phi_2}{\partial x^2}+\frac{\partial^2\phi_2}{\partial y^2}\right)+\Sigma_{a_2}\phi_2=\Sigma_R\phi_1 \tag{20}$$

This equations can be solved analytically and the solution is;

$$\phi_{m,n}(x,y)=\sin\left(\frac{m\pi}{a}x\right)\ \sin\left(\frac{n\pi}{b}y\right) \tag{21}$$

$$B^{m,n}{}_2=\left(\frac{m\pi}{a}\right)^2+\left(\frac{n\pi}{b}\right)^2 \tag{22}$$

$$\lambda_{m,n}=\frac{\nu\Sigma_{f_1}(D_2B^2{}_{m,n}+\Sigma_{a_2})+\nu\Sigma_{f_2}\Sigma_R}{(D_1B^2{}_{m,n}+\Sigma_{a_1}+\Sigma_R)(D_2B^2{}_{m,n}+\Sigma_{a2})} \tag{23}$$

where,

Table 2. Analytic and Numerical Mode Shapes and Corresponding Eigenvalues

mode #	designation (m,n)	eigenvalue (λ_{mn}) analytic	eigenvalue (λ_{mn}) numerical	mode shape $\phi(x,y)=\sin(\frac{m\pi}{a}x)\sin(\frac{n\pi}{b}y)$
1	(1,1)	1.00101	1.00702	+
2	(2,1)	0.62794	0.64039	+ | -
3	(3,1)	0.37728	0.39939	+ | - | +
4	(1,2)	0.36711	0.37842	- / +
5	(2,2)	0.29395	0.30404	+ | - / - | +
6	(4,1)	0.23419	0.26410	- | + | - | +
7	(3,2)	0.22653	0.22992	+ | - | + / - | + | -

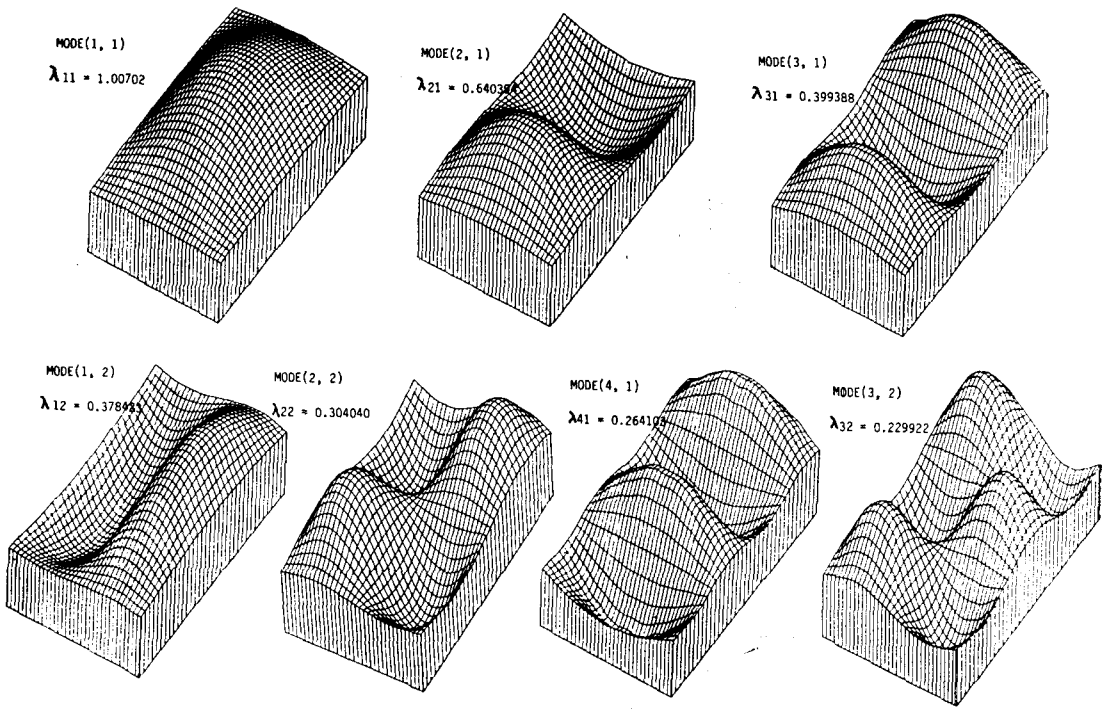


Fig. 2. Numerical Mode Shapes and Eigenvalves

$\phi_{m,n}$=m-th mode in x-direction and n-th mode in y-direction: (m, n) mode

$B^2_{m,n}$=buckling in (m, n) mode

$\lambda_{m,n}$ =eigenvalue in (m, n) mode

Seven modes were calculated by the eq. (21)-(23) and the results are listed in Table 2.

For the same problem, seven modes were calculated by MOGEN and the results is shown in Fig. 2.

The numerical result agree to analytic one within 4% error except the modes (3, 1) and (4, 1). In deriving the 2-group analytic solution, however, we have used the assumption that fast and thermal mode have the same shape. In other 1-group calculation which can be solved analytically without any assumptions, the error was reduced within 0.5%. Therefore, this assumption is the source of error in calculating the analytic eigenvalue.

4. λ-Mode Generation for the CANDU-600 Reactor

We calculated the eight 2-dimensional modes for the CANDU-600 reactor.

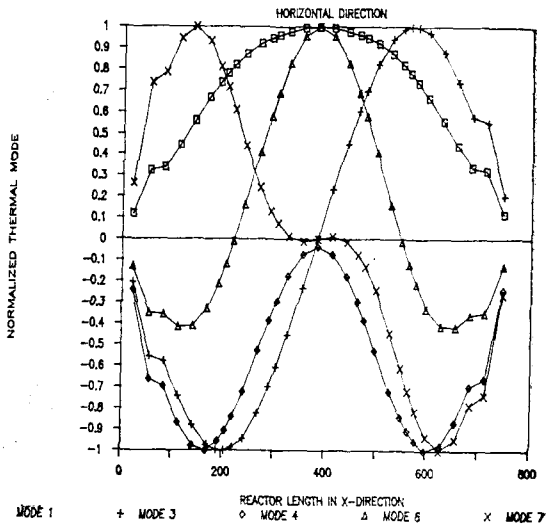
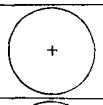
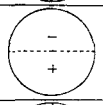
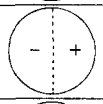
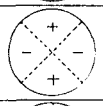
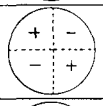
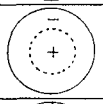
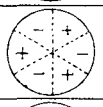
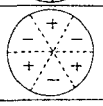


Fig. 3. Mode Distribution at Center of the CANDU-600 Reactor

Table 3. Properties of the 2-Dimensional λ-Modes of CANDU-600 Reactor

No.	Name	Eigenvalue	Mode Shape
1	Fundamental	1.03120	
2	1'st Azimuthal (Top-to-Bottom)	1.00824	
3	1'st Azimuthal (Side-to-Side)	1.00764	
4	2'nd Azimuthal	0.97632	
5	2'nd Azimuthal	0.97513	
6	1'st Radial	0.96071	
7	3'rd Azimuthal	0.93734	
8	3'rd Azimuthal	0.93729	

The reactor model and the material properties which are evaluated by flux weighted, averaging over the reactor length were obtained in reference [7].

Fundamental mode plus other seven higher modes were generated and the properties of these are given in Table 3 and the normalized mode distribution in horizontal direction is shown in Fig. 3.

These modes represent the conventional CANDU mode characteristics well.

5. Application

1) Space-Dependent Kinetics

We can approximate the space and time dependent reactor variables in a finite series of products of unknown time-dependent coefficients, and known space-dependent expansion function. [7]

The calculated λ-modes of the system which makes complete set can be used for this space function, and this method reduce the computing efforts.

2) Approximation for Multi-Dimensional Flux Mapping

The λ-modes can be also used to interpret meaningfully the readings of a number of detectors when each reading depends upon the position of the detectors. [8]

Flux value at an arbitrary position can be expressed as a linear combination of realistic flux shapes, called modes, which span the range of flux distribution to be encountered in the operation of the reactor and mode amplitude which should be determined.

The amplitudes can be calculated by the flux level measured by many in-core detectors.

Actually, the thirteen λ-modes belong to the mode set for flux mapping in CANDU-600 system.

3) Reactor Control Study

As it is impossible to solve all the dynamic equations describing the entire system, the common strategy used in power reactor control is to minimize the flux deviation from some predetermined reference shapes during any transient.

The deviation of the state functions are expressed as a series of the system eigenfunction, and the perturbed equations are solved.

For the stability analysis, the system eigenvalues are checked whether it lies in the left of a complex plane. [6, 9]

6. Summary

The modal expansion technique is suitable for a broad class of space-dependent kinetic problems, flux mapping, and reactor control studies.

The λ-modes which are eigenfunctions of the

reactor system at reference condition are necessary to use this technique.

The computer code MOGEN that generates λ-modes for this purpose was developed.

Futher study should be performed to applicate these harmonics in various reactor problems.

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