Overview of core simulation methodologies for light water reactor analysis

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Abstract: The current in-core fuel management calculation methods provide a very efficient route to predict neutronics behavior of light water reactor (LWR) cores and their prediction accuracy for current generation LWRs is generally sufficient. However, since neutronics calculations for LWRs are based on various assumptions and simplifications, we should also recognize many implicit limitations that are "embedded" in current neutronics calculation methodologies. Continuous effort for improvement of core simulation methodologies is also discussed.

Keywords: neutronics calculation; fuel assembly calculation; core calculation; light water reactors; PWR

1 Introduction

Design of light water reactors (LWRs) essentially relies on simulation methods since design studies based on an experimental approach require impractical cost and design period. Therefore, performance and accuracy of core simulation methods are one of the dominant factors for safety and efficiency of LWRs. In the present paper, current status and of typical core simulation methods for PWRs are reviewed. Furthermore efforts devoted to develop advanced core analysis methods are also described.

The design task of a reactor core is an extensive work, starting from scoping analysis on long term fuel management, scoping design of next cycle, reload core design, analysis of startup reactor physics test, core tracking calculations, on-line core monitoring and so on. Since these tasks are very complicated, various computer codes for simulations are used. These simulation codes are not independent; some of their input may come from output of other codes and output may be used as input for other codes. Namely, simulation codes compose a system, which is a "chain of codes". Since each code contains considerable theoretical backgrounds and numerical algorithms, complete description of a simulation system for LWRs will require a set of whole books. Thus the present paper focuses on typical outline of core neutronics methods for pressurized water reactor (PWR), *i.e.*, a core analysis system, which is usually composed of a lattice code and a core simulation code.

In section 2, overall neutronics calculation flow for PWR will be briefly reviewed. Section 3 and 4 are devoted to descriptions of lattice physics and core calculation methods, respectively. In Section 5, some discussion on the advanced core simulation method is discussed. Conclusion is provided in Section 6.

2 Overall neutronics simulation flow for PWRs

The objective of neutronics design of a reactor core is accurate prediction of core neutronics behavior during operation. Neutronics calculations are based on nuclear data, in which very detail information on neutron reaction probabilities with a target nuclide, *i.e.*, cross sections, is stored for various nuclides. Cross sections in a nuclear data file have fine energy resolution that is sufficient to reproduce complicated behaviors including resonances. For typical heavy nuclides, number of energy grid points to accurately reproduce the original cross section sometimes reaches a few hundreds of thousands.

Theoretically speaking, direct utilization of cross sections with this fine energy representation will give most accurate results. However, such calculation, *i.e.*, a transport calculation with 200,000~300,000 energy groups in three-dimensional whole-core geometry of LWR, is still completely impractical even with today's powerful computers. Of course, we may perform such

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a detail neutronics calculation if we use massively parallel supercomputers. However, it should be remind that many core calculations should be carried out in actual design work as follows.

In order to evaluate a particular status of a core (a state-point), several neutron flux distribution estimations are necessary since we should consider the thermal-hydraulics feedback effect as will be discussed in section 4. For a safety analysis of reload core design, a few hundreds of state-points should be evaluated. In order to develop a loading pattern, dozens to thousands core designs should be evaluated. The above discussion can be roughly summed up as follows:

10^1 (neutron flux calculations/state-point)
$\times$ 10^2 (state-points/a core)
$\times$ 10^2~10^4(cores) =10^5~10^7(neutron flux calculations)

The present rough estimation suggests that at least 10^5 (and may be up to 10^7) neutron flux calculations are necessary for whole process of a reload core design. This fact strictly limits utilization of rigorous methods such as direct utilization of three-dimensional neutron transport calculation with very fine energy groups. For example, the continuous energy Monte-Carlo method offers a pathway to accurately treat a complicated system, but its application is too time-consuming. Instead, many state-of-arts approximations are used in neutronics calculations for reactor core analysis and these approximations are the essence of core simulation methods.

The present neutronics analysis methods put approximations on energetic/angular/spatial behaviors of neutrons in a reactor core. A typical calculation flow used for neutronics design of PWR is shown in Fig.1.

In order to reduce number of energy groups, the multi-groups approach, in which detail energy dependence of cross section in particular energy range is averaged, is used. Starting from a few hundred of thousand energy groups, number of energy groups is finally reduced to a few through several calculation steps.

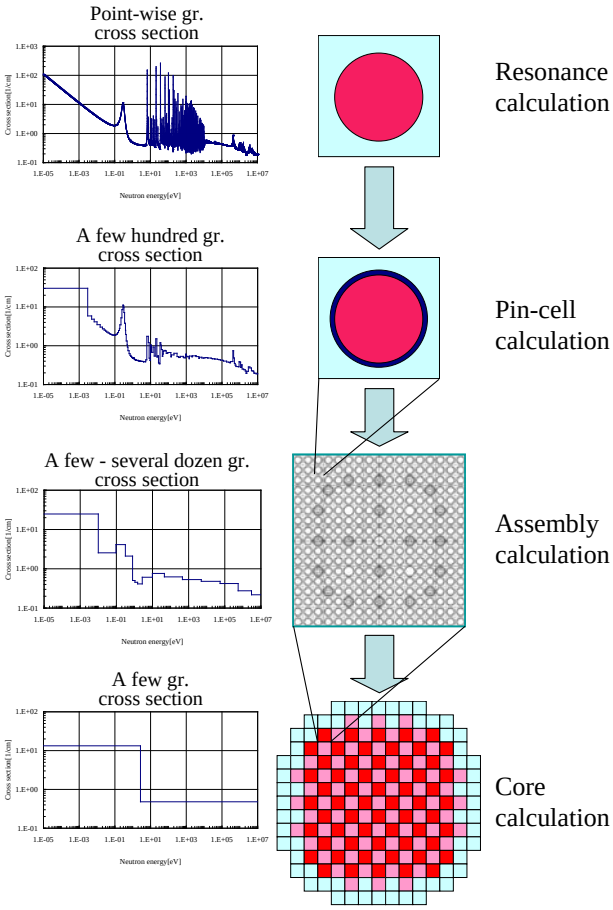


Fig.1 Overall neutronics calculation flow for PWR.

The angular dependence of neutrons is accurately taken into account at the initial phase of calculation chain through the neutron transport theory in heterogeneous geometry. Method of Characteristics is commonly used for fuel assembly calculation and neutron flight direction is discretized into a few hundreds angular points. In the latter phase, the neutron diffusion calculation, which approximately treats angular distribution of neutrons by a truncated expansion of the Legendre polynomials up to the first order (P1), is commonly used for core calculations.

Spatial resolution is gradually reduced from upstream to downstream. In the initial phase, a fine spatial resolution, which can represent complicated and heterogeneous geometry of LWR fuel assembly, is used. Thus typical size of spatial mesh is 1 **mm**. However, coarser spatial discretization is used for core calculations in which detail heterogeneous structure of fuel assembly is homogenized. In this case, spatial mesh size is approximately 10 **cm**.

Generally, in the primary stage of neutronics calculation, energy dependences are accurately treated in a small geometry with zero or one dimensional calculation. In the middle stage, intermediate energy group is used with fine angular and spatial representations, but still in small geometry like fuel assembly. At the final stage, coarser (a few) energy groups with approximate treatments of angular distribution (diffusion theory) and space (homogenization) is used, but whole core geometry is directly treated.

In order to realize the above calculation scheme, neutronics calculation for LWRs is typically divided into three parts. These are the preparation of cross section library for lattice physics computation, the lattice physics calculations and the core calculations. There are several merits to divide a calculation system like this.

The first part, *i.e.*, preparation of a cross section library, is not usually performed in typical LWR core design since a dedicated multi-group cross section library is provided for a lattice physics calculation code. The cross section library generation (preparation) is done to incorporate improvements in nuclear data and to improve cross section library itself, *e.g.*, extension of nuclides stored in the library or increment of energy groups. Thus we can avoid useless repetition of this part by separating the cross section preparation.

In LWRs, specification of a fuel assembly may be fixed for several cycles and may not change cycle by cycle. If we can generate a "general" cross section set, it can be used for several cycles as long as the fuel assemblies with the identical design are loaded. It means that we may skip the cross section generation for a core calculation code, if the second part is separately carried out. Furthermore, preparation of a cross section set should be carried out in prior to core design since it is considerably time consuming and can be carried out when the fuel assembly design is fixed. Note that fuel assembly design is usually specified at least a year before loading due to reading time for manufacturing and transportation.

Finally, since core calculations are repeated many times, its computation time is crucial. By separating generation of a few groups cross section set for core calculation, we can greatly save computation time for core simulation.

Since the second and the third parts, *i.e.*, lattice physics and core calculations, are commonly carried out in typical LWR design, they will be reviewed in the following sections.

3 Lattice physics calculations [1, 2]

3.1 Overview

The objective of the lattice physics computation is generation of assembly homogenized cross section sets in a few groups that are used in a core calculation code. Overall calculation flow of the lattice physics calculation is shown in Fig.2. Since various operating conditions will be considered in core calculations, cross sections generated in lattice physics calculation should cover all operating and shutdown conditions of a reactor. Therefore, series of calculations are carried out to generate a cross section set for a fuel assembly type using a "case matrix". Number of state-points (calculation points) in a case matrix may reach a few to several hundreds in PWR.

3.2 Resonance calculation [1, 2]

Typical number of energy groups of a cross section library for a lattice physics code is several dozen to a few hundreds. However, since variation of cross section (especially resonance part) cannot be exactly captured in such "coarse" groups, average cross section calculated by Eq.(1), which is usually called as the effective cross section, is stored in the cross section library:

$$\sigma_g\left(\vec{r}\right)=\frac{\int_{E_g}^{E_{g-1}} dE\,\sigma(E)\phi\left(\vec{r},E\right)}{\int_{E_g}^{E_{g-1}} dE\,\phi\left(\vec{r},E\right)} \qquad (1)$$

Detail neutron spectrum mainly depends on the magnitude of cross section as show in Fig.3. Since depression of neutron flux also depends on the concentration of resonance nuclide as well as the temperature and neutron inflow from other regions (the heterogeneity effect), the effective cross section is tabulated as a function of temperature and background cross section. Here, the background cross section is a fictitious cross section that represents neutron flux depression at resonance. Detail energy dependence of neutron flux is calculated by the numerical solution of

neutron slowing down equation assuming elastic scattering.

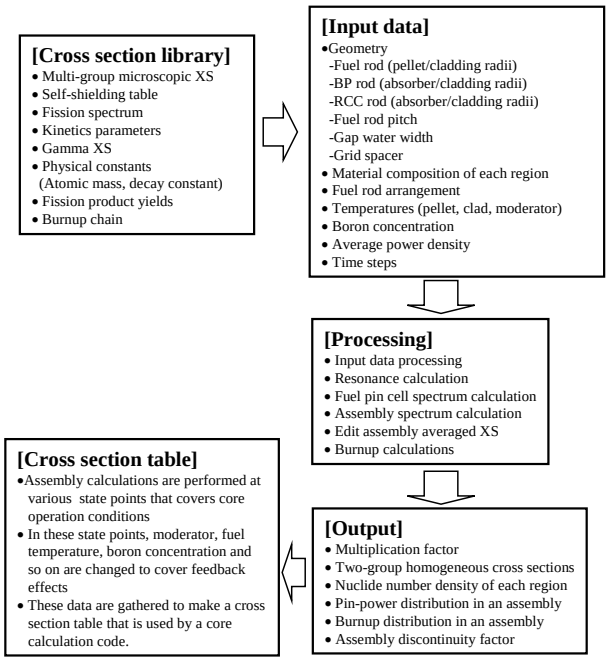


Fig.2 Overall calculation flow of lattice physics calculations.

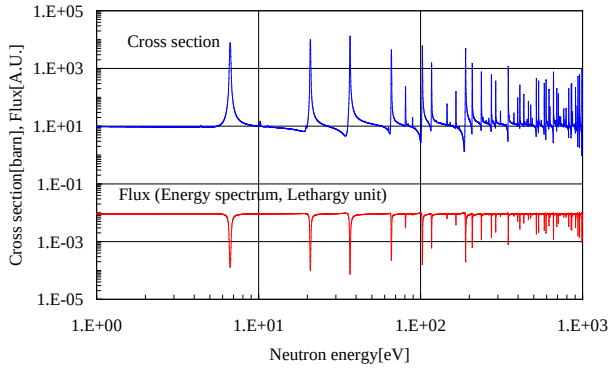


Fig.3 Relation between neutron flux and cross section in fine energy group.

Many lattice physics code adopts the equivalence theory[1] to estimate the effective cross sections. However, other sophisticated methods (*e.g.*, the ultra-fine group method, the sub-group method) are also used in latest lattice physics codes.[3-6]

3.3 Pin-cell calculation [1, 7-9]

Once the resonance calculation is carried out, we have a set of cross sections in library energy groups, which are typically several dozens to a few hundreds. Whole assembly calculation with this energy group is feasible, but it may still time consuming. Therefore, number of energy groups may be reduced through neutron spectrum calculation in small pin-cell geometry. The pin-cell calculation is carried out assuming reflective boundary condition for unit cell and evaluated neutron spectrum is used to collapse multi-group cross sections from library groups to intermediate groups for assembly calculations, which is typically several to a few dozens. The collision probability method is often used for the pin-cell calculation due to its efficiency in small geometry. Note that when shape of a pin-cell (square) is approximated by cylinder to adopt one-dimensional calculation, white boundary condition is applied for cell outer boundary.

In the pin-cell calculation, spectrum interactions among adjacent cells are neglected since the reflective (or white) boundary condition is used. However, in LWR lattice, spatial variation of neutron spectrum in a fuel assembly cannot be omitted due to heterogeneity in an assembly such as water hole and burnable poison. Therefore, number and structure of intermediate energy groups is carefully chosen to accurately capture spectrum interaction in an assembly.

In order to reduce boron concentration and to flatten power distribution in a core, burnable poison is usually used. Since neutron spectrum in burnable poison is significantly different from that in ordinary fuel pin-cell, multi-cell calculation, in which a cell with burnable poison is surrounded by ordinary fuel pin-cells, is carried out to approximately consider the spectrum interaction among them. The guide thimble and the control rod cluster are treated through the similar approach.

3.4 Assembly calculation [10-14]

After the pin-cell calculations, an assembly calculation is carried out to estimate a few group homogeneous cross section of a fuel assembly, which will be used in successive core calculations. In a traditional assembly calculation, heterogeneous structure inside a pin-cell is homogenized though the pin-cell calculation in order to reduce computational burden and the diffusion, the low order (*e.g.* S4) discrete-ordinate or the transmission probability method is used to evaluate space dependent neutron spectrum in an assembly. Though the pin-cell "homogeneous" approach gives reasonable results for the conventional uniform LWR lattice design with low

heterogeneity, its accuracy degrades for advanced fuel assemblies with heavy burnable poison loading (*e.g.*, IFBA, WABA, Gadolinia). Therefore, major lattice physics codes perform more precise transport calculation in heterogeneous geometry with the method of characteristics or current coupling collision probability (CCCP) method. Example of fuel assembly geometry for PWR used in assembly calculation is shown in Fig.4.

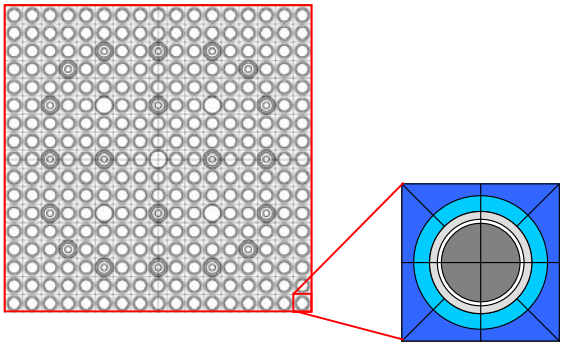


Fig.4 Geometry for fuel assembly calculation of PWR.

The method of characteristics (MOC) is based on the integro-differential form of neutron transport equation in one-dimensional geometry [15-17]:

$$\frac{d}{ds}\psi(s)+\Sigma_t\psi(s)=q\,, \qquad (2)$$

where, s is coordinate along neutron flight direction, $\psi(s)$ is angular flux, Σ_t is total cross section and q is neutron source intensity. In MOC, neutron flight paths (ray traces) are drawn for many directions as shown in Fig.5 and production and absorption of neutrons on each ray trace are evaluated. These production and absorption of neutrons are summed up to estimate neutron balance in each region.

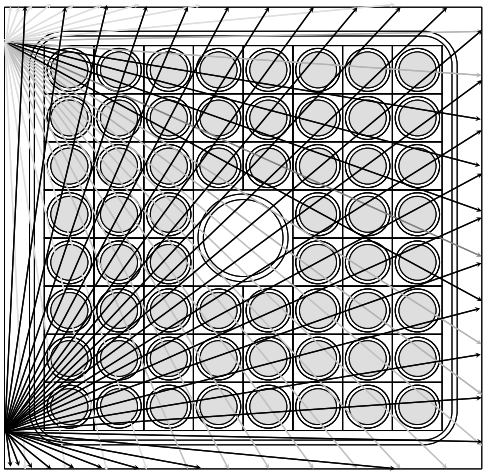


Fig.5 Example of ray trace used in MOC.

Once neutron flux distribution is obtained, we can calculate reaction rates in each fuel pin, which is necessary to evaluate pin-powers and homogeneous cross sections of a fuel assembly.

3.5 Burnup calculation[2, 18, 19]

Variation of nuclide number densities during depletion of fuel assembly is very important for prediction of neutronics characteristics for a reactor core in operation. Burnup calculation is carried out to estimate variation of nuclide number densities in a fuel assembly. The burnup behavior of nuclides in fuel is modeled by burnup chains shown in Fig.6.

General form of the burnup equation is given as follows:

$$\frac{dN_i}{dt}=\sum_j\gamma_{ji}\sigma_{f,j}N_j\phi+\sigma_{c,i-1}N_{i-1}\phi+\sum_k\lambda_kN_k-\sigma_{a,i}N_i\phi-\lambda_iN_i\,, \qquad (3)$$

where,

N_i : number density of nuclide i [1/**cm**^{3}],

γ_{ji} : yield of nuclide i from a fission of nuclide j [-],

$\sigma_{f,j}$: microscopic fission cross section of nuclide j [**cm**^{2}],

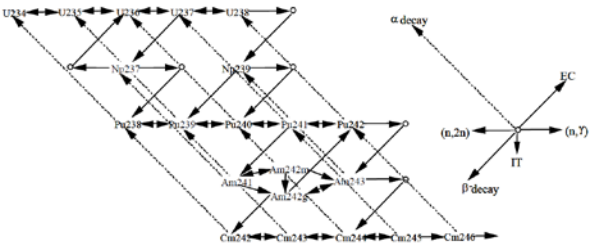
ϕ : neutron flux [1/**cm**^{2}/**sec**],

$\sigma_{c,i-1}$: microscopic capture cross section of nuclide i-1 [**cm**^{2}],

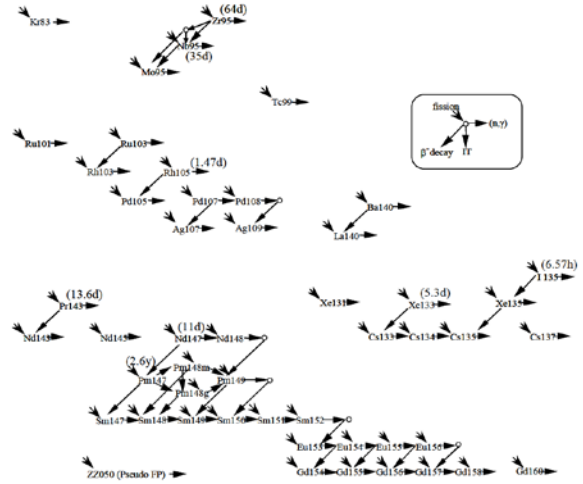
$\sigma_{a,i}$: microscopic absorption cross section of nuclide i [**cm**^{2}].,

λ_i : decay constant of nuclide i [1/**sec**].

Equation (3) can be numerically solved since we know the initial number densities and other parameters through assembly calculation results. Several numerical techniques, *e.g.*, the Runge-Kutta method, the Bateman method, the matrix exponential method, Krylov subspace method are used for burnup calculation. Since these numerical methods have advantages and disadvantages, choice of a numerical algorithm for burnup calculation will be important for accuracy and performance of a lattice physics code.



(For heavy nuclides)



(For fission products)

Fig.6 Example of burnup chains [20, 21]

3.6 Case matrix

In reload core analyses and core tracking calculations, a core calculation code should cover wide range of core situation, *i.e.*, cold shutdown, hot full power operation and may be severe accident with voided condition. Therefore, the lattice physics calculation should prepare a set of cross sections that can cover possible operating, transient and accident conditions.

In order to achieve this, the concept of "case matrix" is commonly used in lattice physics calculations. Though detail of the case matrix depends on the design of a cross section library, example of the case matrix is shown in Table 1. In addition to the burnup calculation, the branch calculations (index number is shown in italic in Table1) are carried out for appropriate burnup steps. Number of burnup steps for depletion calculation may be more than one hundred and number of burnup steps for a typical branch type may be a few dozen. Thus total number of calculation points (state-points) in a case matrix may reach several hundreds. Since lattice physics calculation requires considerable computation time, it is a time consuming task.

3.7 Editing

The objective of fuel assembly calculations is to provide data that is required in successive core calculations. Common data edited from the assembly calculation results are summarized in Fig.2.

Table 1 Example of a case matrix for fuel assembly calculation of PWR [22]

Index	Descriptions	CRD	DEN (g/cm^3)	BOR (ppm)	TFU (K)	TMO (K)
1	Depletion(base)	0	.713	600	820.5	579.5
2	BOR	0	.713	0.1	820.5	579.5
3	BOR	0	.713	1200	820.5	579.5
4	BOR	0	.713	2400	820.5	579.5
5	DEN/TMO	0	.753	600	820.5	559.5
6	DEN/TMO	0	.662	600	820.5	599.5
7	TFU	0	.713	600	559.5	579.5
8	CRD in	1	.713	600	820.5	579.5
9	DEN/TFU/TMO	0	1.01	0.1	293	293
10	DEN/TFU/TMO	0	1.01	600	293	293
11	DEN/TFU/TMO	0	1.01	1200	293	293
12	DEN/TFU/TMO	0	.923	0.1	425	425
13	DEN/TFU/TMO	0	.923	600	425	425
14	DEN/TFU/TMO	0	.923	1200	425	425
15	DEN/TFU/TMO	0	.753	0.1	559.5	559.5
16	DEN/TMO	0	.753	600	559.5	559.5
17	DEN/TFU/TMO	0	.753	1200	559.5	559.5
18	DEN/TFU/TMO	0	.753	2400	559.5	559.5
19	DEN/BOR/TFU/TMO	1	1.01	1200	293	293
20	DEN/BOR/TFU/TMO	1	.923	1200	425	425
21	DEN/BOR/TFU/TMO	1	.753	1200	559.5	559.5
22	SDC(shutdown cooling)	0	.713	600	820.5	579.5
1	Depletion(high mod. dens.)	0	.753	600	820.5	559.5
2	DEN/BOR/TFU/TMO	0	1.01	1200	293	293
1	Depletion(low mod. dens.)	0	.713	1200	820.5	579.5
2	DEN/TFU/TMO	0	1.01	1200	293	293
1	Depletion(low fuel temp.)	0	.713	600	559.5	579.5
1	Depletion(CRD in)	1	.713	600	820.5	579.5
2	CRD out	0	.713	600	820.5	579.5

CRD: control rod, DEN: moderator density, BOR: boron concentration, TFU: fuel temperature, TMO: moderator temperature.

4. Core calculations [23]

4.1 Overview

The final objective of neutronics calculation is accurate prediction of reactor core behavior. Outline of a core calculation in LWR is shown in Fig.7. Reactor conditions (*e.g.*, thermal output, inlet coolant temperature, coolant flow rate, control rod position, boron concentration), geometry (*e.g.*, size of fuel assembly, active length of fuel, fuel assembly arrangement) and fuel loading pattern are given as input data. In addition to these data, a cross section table, which is prepared by editing the assembly calculation results, is also provided to a core calculation code.

4.2 Advanced nodal method [24]

The advanced nodal method, which is based on the diffusion theory, is usually used as a core calculation method. The outline of the advanced nodal method is shown in Fig.8. The direct treatment of detail heterogeneous structure inside fuel assemblies is skipped in order to reduce computation time. Heterogeneous structure inside a fuel assembly is

homogenized through the fuel assembly calculation and pre-tabulated homogeneous cross sections are used in a core calculation. Typical mesh (node) size used in the advanced nodal method is 10 **cm** in radial direction and 20 **cm** for axial direction. In PWR, a fuel assembly is divided into 2x2 nodes in radial direction and ~24 nodes for axial direction. Since mesh size is considerably large, direct utilization of the conventional spatial differencing methods (*e.g.*, the finite-difference method) is impractical due to large spatial discretization error. Instead, neutron flux distribution inside a node is approximated by some functions, *e.g.*, the 4-th order polynomials, sinh, cosh, sin, and cos, part of which are analytic solutions of the diffusion equation.

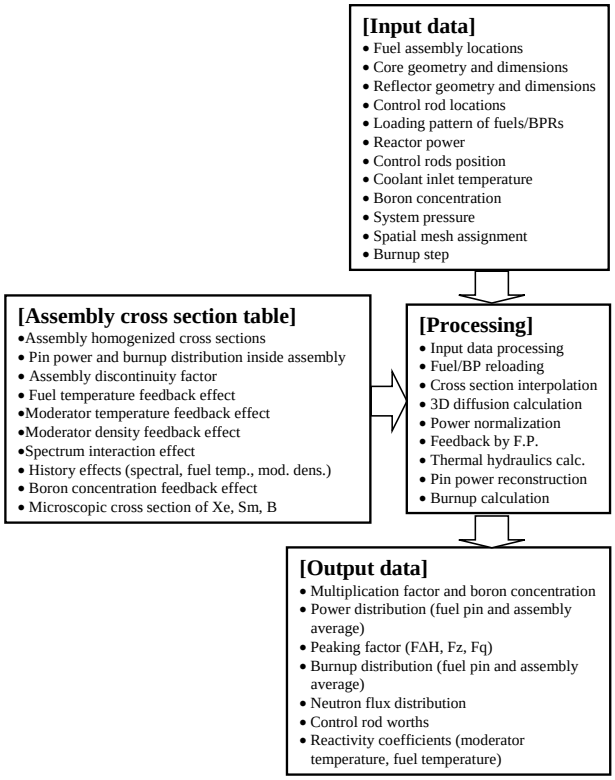


Fig.7 Overall flow of core calculations.

4.3 Feedback effect and interpolation of cross section table

Temperature distribution of fuel and coolant are determined based on the power distribution in a core. However, power distribution and core reactivity are affected by the temperature of fuel and coolant through the Doppler Effect and so on. Variation of coolant density also affects core characteristics through moderation process of neutrons. Therefore, in actual core simulation, neutronics calculation should be coupled with the thermal-hydraulics calculation and a consistent solution that satisfies both neutronics and thermal-hydraulics conditions should be obtained through iteration of neutronics and thermal hydraulics calculations. In PWR, core reactivity is mainly controlled through boron concentration in coolant. The boron concentration is also treated as a feedback effect. Effect of major fission products, ^{135}Xe and ^{149}Sm, may be also treated through the feedback effect.

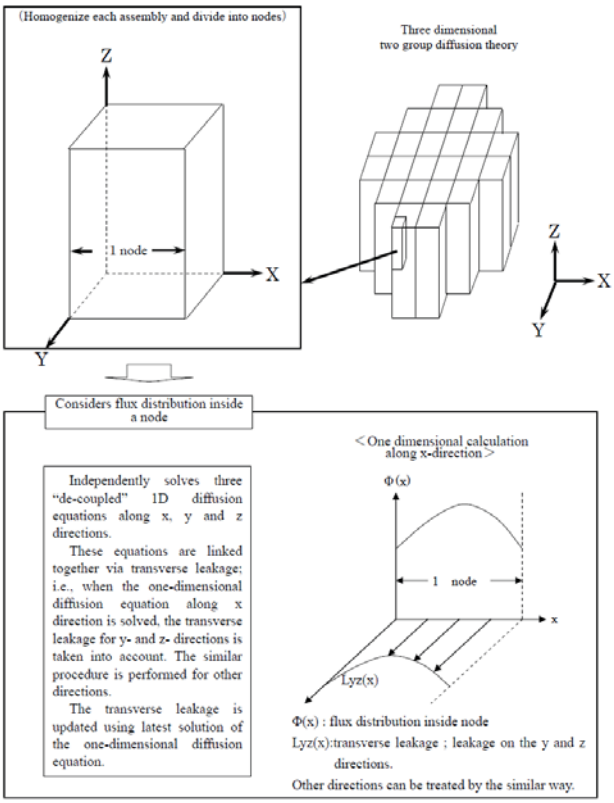


Fig.8 Outline of the advanced nodal method.

In actual core simulation, the feedback effect is taken into account through interpolation of synthesis of cross sections, *e.g.*;

$$\begin{aligned}&\Sigma(EXP,TFU',TMO',CRD',DEN',BOR')\\&=\Sigma(EXP,TFU,TMO,CRD,DEN,BOR)\\&+\Delta\Sigma(EXP,TFU\rightarrow TFU')\\&+\Delta\Sigma(EXP,TMO\rightarrow TMO')\\&+\Delta\Sigma(EXP,CRD\rightarrow CRD')\\&+\Delta\Sigma(EXP,DEN\rightarrow DEN')\\&+\Delta\Sigma(EXP,BOR\rightarrow BOR')\end{aligned}\qquad(4)$$

Cross section is updated according to the temperatures of fuel/coolant, density of moderator and so on. At the initial iteration, uniform temperature may be assumed for all regions in a core then cross sections in each region are interpolated and synthesized using Eq.(4). Neutron flux distribution is obtained through the advanced nodal calculation and first guess of power distribution is obtained using neutron flux. Now the temperature of each region and moderator density can be updated using latest power distribution. These procedures are repeated until convergence.

4.4 Pin-power reconstruction [25]

Pin by pin power distributions are one of the important characteristics in core performances because the thermal limitations such as the maximum linear power density is directly related to the pin power. However, the advanced nodal method utilizes homogeneous cross sections inside a node, thus the pin power distribution cannot be directly obtained from the nodal calculation result.

Therefore, a pin power reconstruction method [25] is utilized to obtain heterogeneous pin power distribution inside assemblies. The pin power reconstruction method synthesizes smooth power distribution and heterogeneous pin power distribution inside an assembly. The smooth power distribution is obtained by the nodal calculation results; flux expansions by polynomials and/or analytic functions are utilized to represent smooth global power distribution inside assemblies. On the other hand, heterogeneous pin power distribution is obtained by assembly calculation results.

By using the advanced nodal method and the pin power reconstruction procedure, core characteristics can be accurately predicted within acceptable computation time. Actually, typical computation time for a depletion calculation of a three-dimensional core (Westinghouse 4 loop type PWR) is approximately several minutes using affordable PCs.

5. Recent advances in LWR analysis

The improvements in fuel design are continuously posing a challenge for core calculation methods used in LWR analysis. Recently, commercial utilization of mixed oxide (MOX) fuel assemblies in both PWR and boiling water reactor (BWR) has been started in Japan. Since neutronics heterogeneity of MOX fuel assembly is much larger than that of conventional UO_2 fuel, more sophisticated core analysis method is desirable for accurate prediction of core characteristics. High burnup fuel also introduces larger heterogeneity due to large water holes, enrichment splitting, and heavy burnable poison loading.

In order to cope the above situation and to catch up the improvements of fuel assembly, various efforts for improvements of core analysis models are being carried out.

In fuel assembly analysis, assembly transport calculations are carried out in library energy groups without cell homogenization, which eliminates energy collapsing error.[26] The higher order anisotropic scattering effect is taken into account since angular distribution in heterogeneous fuel assembly is more skewed, making the effect of anisotropic scattering larger.[26-29]

In core analysis, higher spatial resolution is pursuit by incorporating the pin-by-pin core analysis. In this approach, each fuel pin in a core is explicitly modeled and heterogeneous structure inside a fuel assembly is not homogenized. Furthermore, multi-group (several energy groups) calculations are carried out instead of conventional a few group calculations in order to accurately capture the spectral interaction effect that causes error in neutronics property.[30]

Possibility of so called "on-the-fly" cross section generation is also extensively investigated. In this approach, cross section for core analysis are generated on the demand basis, considering the actual boundary condition of a fuel assembly, *i.e.*, assembly homogenized cross sections are generated using the neutron current obtained by a core analysis code as the boundary condition of lattice physics computation. Major cause of error in the conventional core analysis is the inconsistency of boundary condition in lattice physics computation, in which reflective boundary condition is used. By incorporating the actual neutron current, accuracy of homogenized assembly parameters are increased.[31]

As a more precise method, three-dimensional transport calculation for a whole core with explicit heterogeneous structure is also investigated. In this approach, method of characteristics is extended to a whole core, three-dimensional geometry.[32]

Since the above analysis methods require considerable computation time, efficient utilization of computer hardware is becoming more important issue for core analysis method. Since the present CPU is going to adopt multi-core, multi-threading technology, a numerical algorithm having affinity with such CPU architecture is desirable. Furthermore, non-conventional CPU, *i.e.*, graphic processor unit (GPU), is getting it admiration in the area of scientific computing due to its extreme high capability of parallel computing. If one would like to use full capability of GPU, a dedicated consideration for numerical algorithm is necessary, since the architecture of GPU is somewhat different from the conventional CPU.[33]

6 Summary

Overview of neutronics calculation mainly for PWR is reviewed. Mature, state-of-art neutronics methodologies are used in current in-core fuel management calculations. Since they are based on decades of developments, theoretical backgrounds for some methodologies are complicated and it is difficult to clearly recognize their implicit limitations. Even if we use a software package for in-core fuel management, extensive knowledge and understanding on the methodologies are crucial for safe and efficient operation of a nuclear power plant through core design. In this context, reactor physics is one of the important fundamentals for nuclear power technology though “investment cost” for reactor physics research is not very expensive.

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