Summary of general-purpose reactor physics code system CBZ*

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Abstract

A general-purpose reactor physics code system CBZ is to numerically simulate fission chain reactions in neutron multiplication systems, nuclear fuel depletion (burnup), radiation shielding, transport of neutrons and gamma-ray, and their interaction with nuclei and atom inside and around a nuclear reactor core. This code system has been being developed at the nuclear reactor engineering laboratory of Hokkaido University since April in 2012 based on a code system CBG, which was developed at Japan Atomic Energy Agency.

All programs (source codes) are written in the C++ language, and information (or data) required for reactor physics calculations, such as geometry information describing a reactor core and fuel assemblies, media composing of a reactor core, and numerical methods and conditions, are defined as C++ classes. Several numerical modules which can solve particle transport (or diffusion) equations are implemented, and each of these modules consists of several relevant classes. Data which are exchanged between different modules, such as neutron reaction cross section data and neutron flux data, are defined as instances of these classes, so various types of reactor physics calculations can be easily realized by combining relevant modules in CBZ.

1 A multi-group cross section library, CBZLIB

CBZ is a code system based on the deterministic procedure, so energy variable should be discretized. It means that effective cross section calculations are performed to consider the resonance self-shielding effect. To do that, a multi-group cross section library, CBZLIB, is implemented in CBZ. CBZLIB is what is called the Bondarenko-type reactor group constant, and consists of infinite dilution cross sections, scattering matrices with high-order Legendre coefficients, and resonance self-shielding factors. CBZLIB is produced from evaluated nuclear data files by using processing codes such as FRENDY, and energy group structure is arbitrarily chosen. Generally, a 107-group library, whose structure is the same as the SRAC one, and a 70-group library, whose structure is the same as the JAERI-Fast set, are used for thermal neutron reactor analyses and fast neutron reactor analyses, respectively. Sometimes for fast neutron reactor analyses, a finer group library, a 175-group library, is used [1]

Effective cross section calculations with CBZLIB are done by using self-shielding factors. A set of self-shielding factors is generally calculated under the narrow resonance (NR) approximations in which neutron flux $\phi(E)$ is assumed proportional to inverse of total cross section $\Sigma(E)$. However, in CBZLIB for light water reactor analyses, self-shielding factors of some nuclides are calculated with neutron flux energy spectrum obtained by solving one-point super-fine energy group neutron slowing-down equation. In addition to this, in order to take into account the resonance interference effect between different resonant nuclides, a multiple R-parameter method[1] [2] for heavy nuclides and a simple method to use fixed neutron flux energy spectrum in which resonance interference with uranium-238 is considered[2] for fission product nuclides are adopted. Furthermore, correction factors to improve accuracy of multi-group neutron current-weighted total cross sections are introduced to some specific energy groups of uranium-238 and plutonium-242. We call these resonance treatments as the *advanced Bondarenko method*. Detail of this method is described in Ref. [3].

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[1] Group structure of the 175-group library is called a VITAMIN-J structure, and it was originally proposed for neutron shielding calculations. When small-sized fast reactors with high neutron leakage are calculated, the 70-group library is sometimes not enough accurate, and the 175-group library is preferred.

[2] In resonance calculations of one resonant nuclide, other nuclides are regarded as non-resonant nuclides. However, there are several different resonance nuclides in a medium generally, and an interference effect among different resonant nuclides is important. This effect is referred to as *resonance interference effect*. The R-parameter is defined as a number density ratio of nuclide in consideration to target nuclide to which the resonance interference effect is considered. In the nuclear data file processing, self-shielding factors are calculated on several different values of the R-parameter, and the resonance interference effect to specific nuclide can be approximately considered in resonance calculations.

In CBZLIB, each of nuclide data is defined as a unique text-formatted file. If name of a file is a nuclide name like `Pu239`, it means that this file is generated by the processing codes and neutron flux energy spectrum used as a weighting function in the processing is calculated by the NR approximation. If `T` is attached at the end of a file name like `Pu239T`, it means that neutron flux energy spectrum is calculated by neutron slowing-down equation in the processing, so more accurate calculations can be expected than one whose name does not include `T`. If a nuclide name is attached with a period at the end of a file name like `Pu239.U8`, it means that neutron flux is calculated by slowing-down equation and the resonance interference effect with the specific nuclide can be taken into account by the R-parameter. In this example, the resonance interference effect with uranium-238 is considered because `U8` corresponds to uranium-238. If `.mix` is attached at the end of a file name, it means that proper target nuclides with which the resonance interference effect is considered are chosen for each of energy groups, so the resonance interference effect is taken into account more accurately. The optimized target nuclides are listed in Table 4 of Ref. [3]. Finally, if `.T2` is attached at the end of a file name, it means that this file is generated by using neutron flux in which resonance interference with uranium-238 is considered[2].

2 Resonance calculations

For homogeneous medium, effective cross sections are calculated from infinite dilution cross sections and self-shielding factors. A value of self-shielding factor is determined by interpolation from a self-shielding factor table dependent on background cross section, temperature and R-parameter. On the other hand, for heterogeneous medium, effective cross sections are calculated based on the equivalence theory. Background cross section in heterogeneous medium is calculated as follows; First neutron escape probability from fuel region is calculated by the one-term rational approximation with the Bell factor[4]. Note that the Bell factor is optimized in each energy group for fuel pin-cell of typical light water reactors[1]. Lattice effect or array effect of fuel pins is considered by energy-group dependent Dancoff factors[4]. Tone's method[6], which is familiar in fast neutron reactor analyses, is also available.

Recently, the effective cross sections in homogeneous medium can be calculated directly from ACE-formatted nuclear data files with FRENDY[7]. This scheme is being extended to the hoterogeneous systems[8].

3 Transport and diffusion solvers for neutron and gamma-ray

In CBZ, several modules to solve transport and diffusion equations of neutrons and gamma-rays are implemented. All of them except one are based on one unique base class, a `GeneralSystem` class. This is because numerical procedures such as power iteration or fixed-source calculations can be shared by all these modules. In addition, numerical procedures which use scalar neutron (or gamma-ray) flux, such as reaction rate calculations and part of perturbation calculations, are also implemented in `GeneralSystem`. Adjoint calculations are possible in most of these modules.

There are two modules, `PLOS` and `DHEX`, to solve diffusion equation. These are based on the finite volume method, and `PLOS` can be applied to the Cartesian, cylindrical and spherical coordinates and `DHEX` can be to the hexagonal-Z coordinate. In `DHEX`, triangular mesh division for each of hexagonal mesh is possible. As acceleration methods, the SOR method for inner iteration and the coarse-mesh finite difference (CMFD) acceleration[9] for outer iteration are adopted. In addition to these two, a module `ABEMIE`, which is based on the hierarchical domain decomposition boundary element method[10], is also implemented. ABEMIE can solve diffusion equation defined by arbitrary lines in two-dimension.

There are modules, `SNR`, `SNRZ`, `SNT`, and `SNK`, to solve transport equation. These are based on the discrete-ordinate method and are adopted to sphere systems, cylinder or (r,θ) systems, Cartesian system, and triangular-Z systems, respectively. The discrete-ordinate method treats discrete angular directions of neutron flux, and is generally called the Sn method[11, 12]. Most of these modules adopts acceleration methods: diffusion synthetic acceleration[13] for inner iteration and the CMFD acceleration for outer iteration.

In addition to the above modules, modules `PJI` and `MEC` are implemented to solve neutron transport equation defined on two-dimensional complicated geometry such as fuel pin-cell and assembly. `PJI` is based on the collision probability method[12], and `MEC` is based on the method of characteristic. These modules calculate collision probability or perform neutron flux calculation on characteristics lines by the ray-tracing method[14, 15]. A common module for ray-tracing is used in `PJI` and `MEC`.

CBZ can also solve a simplified P3 (SP3) equation[16, 17]. This is realized by using fixed source calculation capability of PLOS for the Cartesian geometry. Also `ABEMIE` can solve the SP3 equation only for one-group

problems[18].

Generally fission neutron spectrum are treated by a vector form, but it is possible by CBZ to treat fission neutron spectrum as a matrix; incident neutron energy dependence of fission neutron spectrum can be explicitly taken into account.[19]

4 Fuel depletion or burnup calculation

Number densities of various nuclides included in nuclear fuel change with operation of a nuclear reactor. This number density change can be numerically calculated by solving what is called *burnup equation*, and a module tt Burnup does this in CBZ. The matrix exponential method is adopted as a numerical method to solve the burnup equation, and matrix exponential is numerically calculated by the Mini-Max Polynomial Approximation (MMPA)[20, 21] or the Chebyshev Rational Approximation Method (CRAM)[22]. These methods can calculate matrix exponential of burnup problems including nuclides with short half-life, to which the Krylov sub-space method[23] cannot be applied. Also a module `BurnupChainGenerator` which can generate burnup chains is implemented, so arbitrary burnup chains consisting of nuclides chosen by users can be generated from evaluated decay data file and fission yield data file. When one calculates light water reactor fuel burnup problems with CBZ, a chain consisting of 138 fission product nuclides, which are chosen by special algorithm to reproduce reactivity during fuel depletion[24], is recommended to use. A module `Bunrup` calculates nuclide number densities after specified period from initial number densities, neutron flux level and one-group cross section. Information about neutron flux required for one-group calculation are taken from numerical results obtained by transport or diffusion solvers of CBZ.

A `Burnup` module is based on one-group cross section data, but in general burnup calculations, neutron flux energy spectra are calculated, and then one-group cross sections are evaluated and burnup calculations are performed. In CBZ, a base class `GeneralBurner` is implemented to perform burnup calculations of pin-cell problem and multi-cell problems, and this base class is inherited to a module `Burner` for pincell burnup problems and to a module `MulticellBurner` for multi-cell burnup problems[25]. A `Burner` module performs burnup calculations for pincell problem consisting of fuel pellet, cladding and coolant in square or hexagonal infinite array, and a `MulticellBurner` module performs burnup calculations for multi-cell systems in square array. Neutron flux calculations are conducted by the `PJI` module in `Burner` and by the `MEC` module in `MulticellBurner`. Both modules can perform cooling calculations after reactor operation, so they yield various quantities such as nuclide number densities, radioactivity and decay heat during reactor operation and subsequent cooling period. In `MulticellBurner`, the predictor-corrector (PC) method and optimally-weighted PC (OWPC) method[26, 27] are implemented in order to mitigate time discretization error which becomes significant in burnup problems including burnable absorber materials. In addition, fast computation scheme based on the PC method using low-order models is also implemented[28].

In addition to pincell and multicell problems, burnup calculations for a whole core of fast neutron reactors and accelerator-driven systems (ADS) are possible by a module `FRBurnerRZ`[29]. In calculations of `FRBurnerRZ`, fuel assemblies are treated as homogeneous medium and a whole core is simplified to cylindrical geometry. Fuel exchange during multi-cycle operation can also be considered with an approximated manner.

5 Sensitivity and uncertainty analyses

Sensitivity of neutron multiplication factors with respect to nuclear data can be calculated from (forward) neutron flux and adjoint neutron flux, so sensitivities can be calculated by diffusion and transport theories for various problems such as pin-cell, fuel assembly and whole core. Sensitivity of reactivity can be calculated from two sensitivities of neutron multiplication factors. Sensitivity of reaction rate ratios requires generalized adjoint neutron flux calculations[30]. This kind of calculations is fixed-source adjoint calculations, and can be carried out by methods implemented in the `GeneralSystem` class. Sensitivity of parameters whose definition require adjoint neutron flux, such as effective delayed neutron fraction and neutron generation time, can be calculated with a numerical procedure based on a modified k-ratio method[31].

Sensitivities of reactor physics parameters after burnup such as number density, neutron multiplication factor and reaction rate ratio in pincell or multicell problems can be calculated by the depletion perturbation theory[2, 32, 33]. The depletion perturbation theory has been recently extended to burnup calculation with the PC method and the OWPC method[35], and new capability based on this new theory is now available in CBZ.

Sensitivity data are defined in a `SensitivityData` class. Several useful methods are implemented in `SensitivityData`.

Nuclear data-induced-uncertainty quantification calculations are carried out by a module `UNC` using multi-group cross section covariance data and instances of the `SensitivityData` class. Multi-group cross section covariance

data are stored in a specific-format text file, which are obtained from results by the ERRORR module of NJOY-99. Not only cross sections uncertainty but also uncertainties of nuclides decay data and fission yield data can be treated by `UNC`.

6 Neutron and gamma-ray coupled calculation

In case of gamma-ray transport calculations, gamma-ray yield data by neutron-nuclide reactions and gamma-ray transport data (photon-atom reaction cross section data) are prepared from multigroup library which is generated by NJOY-99. When one performs gamma-ray transport calculations in a reactor core, first he has to perform neutron transport equation, and gamma-ray source is calculated from gamma-ray yield data and neutron flux, and then fixed-source gamma-ray transport calculation can be performed. Neutron and gamma-ray coupled calculations with consideration of delayed gamma-ray emission has been realized by CBZ[36]. In the design study on the beam shaping assembly in the medical treatment, this neutron and gamma-ray coupled calculations are utilized also[37].

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