Recent Updates in ETOE-2 and MC²-3

Nuclear Science and Engineering Division

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Recent Updates in ETOE-2 and MC²-3

prepared by

Changho Lee, Hansol Park, Zhaopeng Zhong
Nuclear Science and Engineering Division, Argonne National Laboratory

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ABSTRACT

The MC²-3 code is a multigroup cross section generation code for fast reactor applications, developed by Argonne National Laboratory (ANL) under the DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. In this work, first, the cross section libraries for ENDF/B-VII.1 and ENDF/B-VIII.0 data were generated using the updated ETOE-2 code. Preliminary verification and validation tests of the ENDF/B-VII.1 MC²-3 library were performed with the selected fast reactor benchmark problems. Processing and verifying the libraries suggested that significant efforts would be required for thoroughly verifying the ENDF/B-VII.1 MC²-3 library and successfully processing the ENDF/B-VIII.0 MC²-3 library. Secondly, the cross section generation capability of MC²-3 was updated with the intermediate group lattice calculation and the equivalent Dancoff-factor cell (EDC) method to significantly improve the performance of a two-dimensional assembly calculation using the method of characteristics (MOC). This effort was made useful in implementing and verifying the EDC method in the Griffin cross section API. Finally, we analyzed a SFR problem, for which unusually large deviations in core eigenvalues from Monte Carlo solutions were reported, by generating multigroup cross sections with MC²-3, performing core calculations with DIF3D-VARIANT, and analyzing cross section and eigenvalue results against Monte Carlo solutions. The analysis confirmed that the MC²-3/DIF3D solutions were in good agreement with Monte Carlo solutions, providing the correct process of accurately generating broad-group cross sections with MC²-3.

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1. Introduction

The MC²-3 code [1] is a multigroup cross section generation code for fast reactor applications, developed by Argonne National Laboratory (ANL) under the DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. The code generates region-dependent broad-group (BG) neutron and gamma cross sections by solving one- or multi-dimensional transport equations in ultrafine (~2,000) or hyperfine (~400,000) groups. The code has been verified and validated with various numerical benchmark problems and many fast reactor experiments via the MC²-3/DIF3D-VARIANT [2] code suite, demonstrating good estimation of reference solutions or measurements for most cases [1,3].

This report includes three subjects and updates associated with MC²-3: 1) a MC²-3 library generation using the ETOE-2 code for ENDF/B-VII.1 and ENDF/B-VIII.0 data, 2) a performance improvement in resonance self-shielding for a two-dimensional (2D) method of characteristics (MOC) calculation for cross section generation, and 3) an analysis on the accurate procedure of cross section generation for a sodium-cooled faster reactor (SFR) problem.

So far, MC²-3 has used the cross section library generated based on ENDF/B-VII.0 data, so due to many users' needs, attempts were made in this fiscal year to generate cross section libraries for ENDF/B-VII.1 and ENDF/B-VIII.0 data. Processing ENDF/B-VIII.0 data for the MC²-3 library was more challenging because of an increased number of isotopes (423 isotopes in ENDF/B-VII.1 and 556 isotopes in ENDF/B-VIII.0) and different formats and data in many isotopes of ENDF-VIII.0 data. Since significant efforts are needed to thoroughly perform verification and validation (V&V) of the libraries using a sufficient number of benchmark and measurement data, we initiated generating the MC²-3 libraries with those two ENDF data in this fiscal year and updated the library processing codes RIGEL/ETOE-2 to be able to process the new ENDF/B data.

On the other hand, we have updated the MC²-3 code to improve the performance of its multi-dimensional calculation capability using MOC for cross section generation [4]. First, in order to solve the lattice calculation using MOC using in an intermediate group structure (not in the UFG structure), multiple unit-cell calculations are performed to obtain the UFG weighting spectrum. Second, since the self-shielding calculations based on the MOC fixed-source calculations are very expensive, the equivalent Dancoff-factor cell (EDC) method [5,6] was introduced to improve the calculation performance by replacing a 2D assembly fixed-source problem with multiple decoupled 1D slowing-down problems. This dramatically improved the calculation performance because 1D calculations using CPM are much faster than a 2D assembly fixed-source calculation using MOC. This effort was later very useful in verifying the EDC method prior to implementing it to the Griffin cross section API (CSAPI) [7].

Recently, it has been reported in conference papers [8,9] that the MC²-3/DIF3D analysis for an SFR problem resulted in noticeable differences (> 500 pcm) in eigenvalue from Monte Carlo solutions. In order to review these results independently, we analyzed the same SFR problem by generating multigroup cross sections with MC²-3 and performing core calculations with DIF3D-VARIANT (hereafter DIF3D). To investigate the potential reasons for the reported large eigenvalue

deviations, a set of broad-group (BG) cross sections were generated using different spatial calculational models of MC²-3. Finally, DIF3D core calculations were performed with these cross section sets, whose results were compared with Monte Carlo solutions.

In this report, Section 2 presents the generation of new MC²-3 libraries, Section 3 discusses the updates made to MC²-3 for cross section generation, and Section 4 details the analysis results of MC²-3/DIF3D for a SFR benchmark problem. Conclusions are made in the last section.

2. Updates in MC²-3 Libraries

Attempts were made to process two new ENDF data for MC²-3 libraries. Processing the ENDF/B-VII.1 data, which includes 30 more isotopes than ENDF/B-VII.0 data, was overall successful, while many issues were found in generating the MC²-3 library with ENDF/B-VIII.0 data. This section presents library processing and preliminary verification tests of the produced libraries.

2.1 MC²-3 Library Processing Codes

The RIGEL and ETOE-2 codes are used to generate a MC²-3 neutron reaction library, processing ENDF/B data which contains evaluated data in the form of six data records. First, the RIGEL code reads isotopic ENDF/B data and transforms them from the ENDF/B format into the binary format which is readable by ETOE-2. In this step, basically no change is introduced in the original structure of the ENDF/B file. The ETOE-2 code processes a binary format of nuclear data written by RIGEL to produce eight binary library files for use in MC²-3.

The ETOE-2 code performs the following five basic functions which are diagrammed in Figure 2.1: (1) reformat the data, (2) preprocess resonance cross sections by converting Reich-Moore parameters to multi-pole parameters, (3) generate ultrafine-group smooth cross sections, (4) calculate isotope-independent function tables, and (5) convert all ENDF/B formats to the laws which are allowed in MC²-3.

Figure 2.1 Generation of Isotopic MC² Library in ETOE-2

The ETOE-2 code is able to treat common resonance formalisms such as the single level and multilevel Breit-Wigner formulas, the Adler-Adler description, and the Reich-Moore formalism. Among them, the Reich-Moore parameters are converted to multi-pole parameters or Adler-Adler parameters so that cross sections at any energy and temperature conditions can be represented as a

linear combination of the Doppler-broadened line shape functions. This is necessary for analytic Doppler broadening on the fly in the cross section generation in MC²-3.

While the ENDF/B data permit six secondary energy distribution laws for inelastic and (n,2n) scattering reactions, MC²-3 permits only three of those: tabulated function, evaporation spectrum, and discrete levels, and thus ETOE-2 generates a tabulated function for data which are provided with other than the three laws.

The binary data files provided by the ETOE-2 code contains resolved resonance parameters, unresolved resonance parameters, ultrafine group smooth cross sections, inelastic and (n,2n) scattering data, fission spectrum parameters, elastic scattering distributions, isotope-independent function tables, and an administrative file. Those data are saved in the MC² library files as listed in Table 2.1.

Previously, the ETOE-2 code was significantly updated in order to correctly process the ENDF/B-VII.0 data previously. Further updates have been made to process the ENDF/B-VII.1 data since many issues were encountered when processing some of the new isotopes added to the ENDF/B-VII.1 and the existing isotopes with a significant addition of data.

Among eight MC²-3 libraries (MCCF1 – MCCF8), MCCF2 contains isotope-independent function tables, which does not change with ENDF/B data. The rest seven library files are generated from ETOE-2, for which isotopic files are first produced and then merged to seven single files for MC²-3 to read. In future, MC²-3 may need to be updated to allow individual isotopic library files to make it easy to fix isotopic issues and simplify the data searching and reading process in the code.

Table 2.1 MC² Library Files

Library	Description
MCCF1	Maximum data sizes, control information, material IDs, etc.
MCCF2	Isotope-independent function table
MCCF3	Unresolved resonance data
MCCF4	Resolved resonance data
MCCF5	Ultrafine-group smooth (non-resonant) cross section data
MCCF6	Inelastic and (n,2n) P ₀ scattering data
MCCF7	Fission spectrum, neutron-per-fission data
MCCF8	T-function matrices, anisotropic elastic scattering Legendre data
MCCF9	Chi matrix, infinite-dilute ultrafine-group total cross sections
MCCF10	Ultrafine-group Inelastic scattering matrices

MCCF9 contains fission spectrum matrices and infinite-dilute ultrafine-group (UFG) total cross sections, while MCCF10 involves UFG inelastic scattering matrices up to P1. Those two libraries are generated directly from NJOY GROUPR [10] because ETOE-2 provides fission spectrum vectors and P0 inelastic scattering matrices only.

In MCCF9, the fission spectrum (“chi”) matrix data are stored in a form of the UFG chi matrices as a function of incident and secondary neutron energies for fissionable isotopes. In MCCF10, the inelastic scattering data are saved in the UFG matrix form of P_0 and P_1 inelastic scattering reactions. Since the P_0 inelastic scattering data are also included in MCCF6, the P_1 inelastic scattering data in MCCF10 are updated based on the normalization of the P_0 data to be consistent with those in MCCF6 when MC²-3 calculations are performed.

Like the other MC²-3 libraries, the isotopic data of MCCF9 and MCCF10 are generated individually and merged to single library files in the same isotopic order saved in MCCF1. The summarized library generation process is illustrated in Figure 2-2.

Figure 2-2. Procedure of the MC²-3 Library Generation

MC²-3 allows to read the PENDF files generated from NJOY as well, which are used as an alternative to reconstruct point-wise resolved resonance cross sections or to self-shield the resonance-like cross sections of intermediate mass isotopes above the resonance energy. Note that the MC²-3 library include data for reconstructing pointwise cross sections in the resonance energy range only, and therefore the PENDF data allow us to reconstruct pointwise cross sections outside the resonance energy range.

2.2 ENDF/B-VII.1 Library

2.2.1 Library Generation

Compared to the ENDF/B-VII.0 data, 30 more isotopes are included in the ENDF/B-VII.1 data. The MC² libraries are prepared for almost all 423 isotopes of ENDF/B-VII.1. The resolved and unresolved resonance energy ranges of all isotopes are summarized in Figure 2-3. Basically, resonance energy ranges are increased, compared to the previous ENDF data.

The ENDF/B-VII.1 library of MC²-3 were generated using RIGEL/ETOE-2 as well as NJOY as discussed in the previous section. Most of the isotopes were generated successfully, but several isotopes are currently not provided to the library. As listed in Table 2-2, Tm-168 and Cf-251 are not included in the main library files, and fission spectra and inelastic scattering cross sections for several minor isotopes are missing in the MCCF9 and MCCF10 files. Those missing data will be updated in future.

Figure 2-3. Upper Energy Boundaries of Resolved and Unresolved Resonances of ENDF/B-VII.1 Data (423 Isotopes)

Table 2-2. Incomplete Isotope Data in the ENDF/B-VII.1 MC²-3 Library

Library	Missing Data
MCCF1-8	Tm-168, Cf-251
MCCF9	Chi for U-241, Es-251, Es-252, Es-254m Infinite-dilute total cross sections for Zn-65, Pm-148, Eu-156
MCCF10	Inelastic scattering for Ni-59, Zn-65

2.2.2 Verification

Preliminary verification tests were performed for the ENDF/B-VII.1 MC²-3 library. First of all, using a simple homogeneous composition, the infinite-dilute total microscopic cross sections of all isotopes in the 230-group structure were generated from MC²-3 and NJOY, which were compared with each other. Even though noticeable deviations were observed for many isotopes, the infinite-dilute total cross sections for major isotopes (12 selected isotopes) resulted from the two codes were mostly in good agreement within 0.5%, as shown in Figure 2-4. Among them, those of Fe-56, Ni-58, Mo-98, and Pu-241 showed noticeable differences of up to 3% in some energy groups in the range of 34 – 865 keV. It was found that several tens of isotopes had large differences in total cross sections, as shown in Figure 2-6. Those isotopes with noticeable differences will be further investigated in future. Thorough verifications will be conducted as well, inspecting all partial cross sections in various self-shielding and temperature conditions.

For integral tests, fast reactor benchmark problems were calculated using the new library, which include six eight LANL critical assemblies, ZPR-6 Assemblies 6A and 7, three loadings of ZPPR-15A, six phases of ZPPR-21, Monju start-up core, and ABTR (Advanced Burner Test Reactor). Additional benchmark problems were created by simplifying several critical experiments to RZ

geometries or using simple homogeneous unit cells. Reference solutions for those numerical benchmark problems were obtained from MCNP Monte Carlo calculations.

For deterministic calculations, 230-group isotopic multigroup cross sections were generated using MC²-3. One-dimensional unit-cell calculations were performed for ZPPR-15 problems, which have heterogeneous fuel drawers, to account for the heterogeneity effect in the cross sections. The TWODANT code was used for RZ geometries, and the DIF3D code was used for the 3D Cartesian and hexagonal geometry problems (ZPPR-15 and ABTR). All TWODANT calculations were performed with an angular quadrature of S₂₄ and an anisotropic scattering order of P₃. The DIF3D calculations for ZPPR-15 were performed using the nodal transport option, equivalent to S₄ angular quadrature and P₁ scattering approximation. For the ABTR problem in Hex-Z geometries, the VARIANT option in DIF3D was used with P₅ angular flux approximation and an anisotropic scattering order of P₃.

Figure 2-4. Percent Differences between MC²-3 and NJOY in 230-group Infinite-dilute Total Cross Sections of ENDF/B-VII.1 Major Isotopes

Figure 2-5. Maximum % Differences between MC²-3 and NJOY in 230-group Infinite-dilute Total Cross Sections of ENDF/B-VII.1 Isotopes

Figure 2-6 compares MCNP solutions between using ENDF/B-VII.0 and VII.1 data to see the effects of the libraries on the benchmark problems, indicating that the ENDF/B-VII.1 data made the eigenvalues of the benchmark problems change by up to ~250 pcm, mostly smaller than the solutions with the ENDF/B-VII.0 data.

Figure 2-7 shows the core eigenvalues obtained with the ENDF/B-VII.1 libraries which are in good agreement between MCNP and deterministic solutions (DIF3D or TWODANT). This indicates that the ENDF/B-VII.1 library of MC²-3 was generated reasonably. However, noticeable differences in core eigenvalue between the two ENDF/B libraries were observed for some ZPPR-21 phases and the Monju case. The dominant contributors to those differences will be investigated in future.

Using the ENDF/B-VII.1 library, MC²-3/DIF3D calculations were performed for the experimental cases for six phases (A-F) of ZPPR-21 and three loadings (15, 16, and 20) of ZPPR-15. The ZPPR-21 assembly, shown in Figure 2-8 (left), consists of a series of six criticality benchmark cores built in the ZPPR facility to provide data for validating criticality calculations for systems. The assemblies were graphite reflected, and different mixtures of plutonium and uranium were used in mock-up Pu-U-zirconium fuel. The first configuration, ZPPR-21A, was built with only plutonium fuel to take advantage of the inherent neutron source of Pu-240. Then, enriched uranium was progressively substituted for plutonium in Phases B through E. The final configuration, ZPPR-21F, had an all-uranium fuel loading and required an external neutron source to assist in the approach to critical.

ZPPR-15 Phase A, shown in Figure 2-8 (right), was a clean physics assembly containing only plutonium, depleted uranium, stainless steel and sodium without zirconium, which was progressed to the succeeding phases by adding zirconium to the core composition. Three loading configurations of the ZPPR-15 phase A experiments involve the initial criticality configuration (loading 15), a reference configuration for sodium void worth measurement (loading 16), and a configuration with an 18-inch sodium void in part of the inner core (loading 20).

Figure 2-9 shows that MCNP and MC²-3/DIF3D core eigenvalues are in good agreement and most of the calculated core eigenvalues using the ENDF/B-VII.1 data are closer to the measurements than those using the ENDF/B-VII.0 data. Note that 1 σ uncertainties of the measured core eigenvalues of ZPPR-21 and ZPPR15 loadings 15, 16, and 20, which are 230-260 pcm and 180 pcm, respectively. Further detailed and integral verification tests are needed for the ENDF/B-VII.1 MC²-3 library, which will be conducted in future.

Figure 2-6. Comparison of Eigenvalues between MCNP Solutions with ENDF/B-VII.0 and ENDF/B-VII.1 Data for Fast Reactor Benchmark Problems

Figure 2-7. Comparison of Eigenvalues between MCNP and MC²-3/DIF3 (or TWODANT) with ENDF/B-VII.1 Data for Fast Reactor Benchmark Problems

Figure 2-8. Benchmark Model Geometry for ZPPR-21A (left) and ZPPR-15A Loading 15 (right)

Figure 2-9. Comparison of k-effective Solutions of MCNP and MC²-3/DIF3 with ENDF/B-VII.1 Data against ZPPR-21 and ZPPR-15 Measurements

2.3 ENDF/B-VIII.0 Library

Compared to the ENDF/B-VII.1 data, 133 more isotopes are included in the ENDF/B-VIII.0 data. The resolved and unresolved resonance energy ranges of isotopes in the ENDF/B-VIII.0 data are illustrated in Figure 2-10. This year, we initiated generating the MC2-3 libraries for ENDF/B-VIII.0 data. A noticeable change of formats in the new data required us to further update the library processing code RIGEL/ETOE-2. For MCCF9 and MCCF10 which include UFG-based inelastic scattering matrices, fission spectra and infinite-dilute total cross sections, the 2016-version of NJOY should be used.

Among total 556 isotopes, the isotopic MC²-3 libraries for most of the isotopes, except for 61 isotopes that are rarely used, appeared to be successfully generated using the updated RIGEL/ETOE-2. As shown in Figure 2-11, 230-group infinite-dilute total cross sections of some major isotopes agreed well with those produced from NJOY. However, while testing the MC²-3 libraries, many issues were found, including problems in unresolved and resolved resonances, inelastic scattering cross sections, etc. Even in Na-23, Cr-50, and Ni-58 (Figure 2-11), for example, relatively large differences in total cross sections between MC²-3 and NJOY were observed in the energy range of 500 – 820 keV, which were not shown in the ENDF/B-VII.1 MC2-3 library.

Overall, we realized that processing the ENDF/B-VIII.0 data for MC²-3 was not trivial since significant changes were made to the data, compared to the previous ENDF data. Substantial efforts are expected to investigate and resolve the issues discovered this year. Based on the lessons learned from processing the ENDF/B-VIII.0 data in this fiscal year, we will continue to work on processing the ENDF/B-VII.0 MC²-3 library in the following year. An alternative way of generating all the MC²-3 library files using NJOY, instead of ETOE-2, will be investigated as well.

Figure 2-10. Upper Energy Boundaries of Resolved and Unresolved Resonances of ENDF/B-VIII.0 Data (556 Isotopes)

Figure 2-11. Percent Differences between MC²-3 and NJOY in 230-group Infinite-dilute Total Cross Sections of ENDF/B-VIII.0 Major Isotopes

3. Updates in MC²-3

Several updates have been made to MC²-3 for the cross section generation capability [4] in which the original low energy limit of 0.414 eV is extended to 10^{-5} eV. The thermal energy range from 5.002 eV to 10^{-5} eV is represented by 1,700 ultrafine groups (UFGs) of unequal lethargy widths, and the fast energy range from 14.19 MeV to 5.00 eV is divided into 1,783 UFGs of equal lethargy width of 1/120. For cross section generation of thermal spectrum problem, detailed heterogeneous lattice calculation should be performed due to very small neutron mean free path. Since solving the 3,483-group (UFG) eigenvalue problem and the hyperfine group (HFG – 416,400 groups) slowing down problem using the 2D MOC in an exact heterogeneous lattice geometry are too demanding, practical measures were introduced. First, a user-defined UFG unit-cell problem is solved to obtain a weighting spectrum for condensation into an intermediate group (IG) structure in which a lattice calculation is performed. Second, the equivalent Dancoff factor cell (EDC) method was employed to improve the performance of the HFG slowing down calculation as well as to verify the method before implementing to the cross section API (CSAPI) [5]. These two measures are explained in detail in this section.

3.1 Intermediate Group Lattice Calculation

For thermal cross section generation, the code was updated in a way that a default calculation mode is the lattice calculation in a user-defined IG structure. To generate multigroup cross sections in the IG structure, unit-cells can be defined by a user to obtain a weighting spectrum. Unit-cells are defined in a cylindrical geometry with the white boundary condition and the 1D CPM solver is used to solve the eigenvalue problems in the UFG structure. A user should map which region spectrum is to be used to condense cross sections in which MC²-3 regions. Once UFG spectra are obtained, multigroup cross sections in the IG structure are obtained and used in the 2D MOC lattice calculation in the IG structure.

3.2 Implementation of the Equivalent Dancoff-factor Cell Method

This method belongs to the on-the-fly slowing down method as one of the resonance self-shielding method in a lattice physics code for thermal spectrum problems. Since performing the slowing down calculation using the 2D MOC in an exact heterogeneous lattice geometry is too demanding, an approximation is introduced to geometry and transport calculation scheme. The heterogeneous lattice geometry is decoupled to multiple 1D pin-cell problems that preserve the Dancoff factor calculated in the reference geometry using the 2D MOC solver. The Dancoff factor for each fuel pin is obtained using the enhanced neutron current method (ENCM) [12], and the equivalent outermost radius of 1D cell of each fuel pin is obtained using the binary search to give the identical Dancoff factor obtained by using the 1D CPM. This 1D cell is called the equivalent Dancoff factor Cell (EDC). Then, the slowing down problem is solved in the EDC using the 1D CPM. This approach is basically based on the same idea used in the SCALE procedure that the SCALE Monte Carlo code MCDancoff is used to compute Dancoff factors, which are then used to modify the standard CENTRM two-region 1D unit cell models to account for 3D lattice heterogeneous effects

[5]. This approach was successfully demonstrated for a pressurized water reactor (PWR) assembly problem by another code named Galaxy as well [6].

3.3 Computational Procedure

The brief picture of the overall default calculation procedure is shown in Figure 3-1. First, a Dancoff factor for each fuel pin is calculated using the ENCM and the EDC for each fuel pin is determined. Then, UFG weighting spectrum is obtained by solving a user-defined UFG unit-cell problem by following the UFG/HFG calculation procedure of MC²-3 and used for condensation to obtain IG cross section for each region. If there exist stochastic regions, just volume homogenized composition is used for the unit-cell calculation and resulting IG cross sections of the composition are saved for all its micro-regions. Note that the order of these first two steps does not matter. If stochastic regions exist, compact-averaged cross sections are obtained using the iterative local spatial self-shielding (ILSS) method [13] as an IG quantity for the fast and thermal energy ranges and as a HFG quantity for the resonance energy range. Otherwise, this step is skipped. Then, the HFG slowing down problem for each fuel pin is solved in its EDC and compact-averaged effective IG cross sections for the resonance energy range are updated. Using these compact-averaged IG effective cross sections for the whole energy range, a lattice IG transport calculation is performed to generate cross sections in a target group structure for downstream codes.

Figure 3-1. Thermal Cross Section Generation Procedure of MC²-3 for Particulate Fuels

3.4 Verification

The implemented procedure was verified for 2D assembly problems derived from the High Temperature Test Reactor (HTTR) configuration [14]. The assembly configuration selected for verification is shown in Figure 3-2 with actual meshes used in 2D MOC calculations of MC²-3. It is a 31-pin 6.3 wt.% UO₂ fuel assembly located in Zone 4 at the periphery of the core with two 2.5 wt.% B₄C burnable poison (BP) rods inserted in two out of three BP insertion holes and a fuel handling hole at the center. Two problems were solved: one with two BP rods inserted and the other one with BP rods fully withdrawn. The fuel rod is the A-type fuel with 30.0% packing fraction of TRISO particles (13000 particles of radius of 0.046 cm in 3.9 cm height annular compact of inner radius of 0.5 cm and outer radius of 1.3 cm). A room temperature of 293.6 K was assumed for all problems.

Figure 3-2. Geometry and Mesh Used in MC²-3 Calculation for 2D HTTR Assembly Problem.

For Serpent2 [11] reference solutions, 31 different random particle locations were used in each fuel pin and randomly shuffled 10 times for 10 independent Serpent2 runs, and the averaged value for 10 results was taken as the reference solution. For each run of heterogeneous compact problems, 10^5 particles/cycle, 100 active and 100 inactive cycles were used, and for homogenized compact problems, 10^5 particles/cycle, 1000 active and 100 inactive cycles were used. For MC²-3 calculations, each annular fuel compact and each B₄C rod were divided into 3 and 9 radial meshes of equal volume with one cross section zone, respectively, while graphite sheath and block were divided into the enough number of meshes, as shown in Figure 3-2. MOC calculations were performed using 66 azimuthal angles per 180°, 4 Tabuchi-Yamamoto optimum polar angles [15], and ray spacing of 0.02 cm with P₂ anisotropic scattering order. A convergence criterion of 10^{-6} was used for both eigenvalue and fission source.

A new 68-group structure was derived to have the smallest eigenvalue errors over a wide range of spectra for a graphite-moderated system with a fresh uranium fuel and used as the intermediate group structure. There are 32 fast and 36 thermal energy groups with the boundary of 5 eV. It has

almost uniform lethargy widths above 10 eV. An energy range near the U-238 resonance at 6.67 eV is divided into several groups because the U-238 effective capture cross section between 5 eV and 9 eV is overestimated by $\sim 3\%$ due to the neglect of graphite up-scattering above 5 eV in the HFG slowing down calculation, which induced reactivity bias bigger than about -100 pcm.

For IG calculation, the code starts with the UFG eigenvalue calculation in a unit-cell to obtain a UFG weighting spectrum for condensation to the IG structure. Figure 3-3 shows the 1D unit-cell on the left and the comparison of the UFG spectra obtained from the MC²-3 unit-cell calculation and Serpent2 calculation on the right. The unit-cell was constructed by keeping the internal geometry of the fuel unit-cell of the lattice and determining the outermost radius of the graphite region to preserve the relative amount of graphite with respect to the amount of fuel in the lattice. The UFG spectrum of the fuel region in the unit-cell calculation (bold black) is approximately matching the average UFG spectrum in the fuel regions obtained from the Serpent2 calculation in the B₄C unrodded case (blue), and is used as a weighting spectrum for the fuel region in both the B₄C unrodded and rodded cases and the B₄C region. Weighting spectra for graphite and helium gap regions were taken from the spectrum solution at the corresponding regions in the unit-cell calculation although not shown explicitly in Figure 3-3.

Figure 3-3. Unit-cell Model (left) in MC²-3 for Obtaining UFG Weighting Spectrum, Resulting Weighting Spectrum (right) of MC²-3 and Fuel and B₄C Spectra of Serpent2 for Actual Problems.

Eigenvalue results for the homogeneous and heterogeneous compact problems of B₄C unrodded and rodded cases are compared in Table 3-1. In the Serpent2 results for the double heterogeneous problems, there are two uncertainties: the first indicates the average value of 10 standard deviations and the second indicates the standard deviation of 10 quantities. For the power result, RMS (root mean square) and maximum values show statistics of those values among the 31 pins. For the B₄C unrodded case, the UFG/2D MOC HFG scheme shows reactivity errors of -66 and -15 pcm for

homogenized and heterogeneous compact problems, respectively, and the UFG/EDC HFG scheme shows the identical results. Although not shown, the UFG cross sections are identical, which indicates that the EDC method works perfectly well in the UFG structure. The FG/EDC HFG scheme shows almost identical results with the other two cases with 10 and 1~2 pcm differences for homogenized and heterogeneous compact problems, respectively. For the B₄C rodged case, the UFG/2D MOC HFG scheme shows reactivity errors of -141 and -93 pcm for homogenized and heterogeneous compact problems, respectively, and the UFG/EDC HFG scheme shows the identical results. The FG/EDC HFG scheme shows +28 and +45 pcm differences for homogenized and heterogeneous compact problems, respectively, compared to the UFG/2D MOC HFG scheme.

Table 3-1. Comparison of Eigenvalue and Pin Power of MC²-3 with Those of Serpent2 for 2D HTTR Assembly Problems w/ and w/o B₄C Burnable Poison Rods

Problem: w/o B ₄ C		Homogenized Compact				Heterogeneous Compact			
Code/Scheme		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)	
				RMS	MAX			RMS	MAX
Serpent2		1.50820	±4	±0.04	±0.05	1.53375	±13 ^a ±21 ^b	±0.18 ^c ±0.19 ^d	±0.19 ^c ±0.33 ^d
MC ² -3	UFG 2D MOC HFG	1.50671	-66	0.24	0.36	1.53339	-15	0.25	0.38
	UFG EDC HFG	1.50669	-66	0.24	0.36	1.53337	-16	0.25	0.38
	FG EDC HFG	1.50640	-79	0.18	0.26	1.53341	-14	0.18	0.29
Problem: w/ B ₄ C		Homogenized Compact				Heterogeneous Compact			
Code/Scheme		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)		K-eff	$\Delta\rho$ (pcm)	ΔP_{pin} (%)	
				RMS	MAX			RMS	MAX
Serpent2		1.25001	±7	±0.04	±0.04	1.26976	±19 ±27	±0.18 ±0.19	±0.19 ±0.33
MC ² -3	UFG 2D MOC HFG	1.24780	-141	0.29	0.45	1.26826	-93	0.33	0.56
	UFG EDC HFG	1.24779	-142	0.29	0.45	1.26825	-94	0.33	0.56
	FG EDC HFG	1.24823	-114	0.22	0.37	1.26897	-49	0.27	0.48

a) Average of 10 eigenvalue standard deviations, b) Standard deviation of 10 eigenvalues

c) RMS and MAX for averages of 10 standard deviations of each pin power

d) RMS and MAX for standard deviations of 10 pin power values

Figure 3-4 shows relative errors of U-238 capture cross sections computed by the 2D MOC HFG calculation and the EDC HFG calculation at pins 3, 9, 14 and 16 in Figure 3-2, for both homogenized (single het.) and heterogeneous (double het.) compact problems of the B₄C unrodged case. Cross section errors are all within ±2% except at 6.67 eV resonance for heterogeneous compact problems. Cross sections computed by the EDC HFG calculation are slightly smaller than

those computed by the 2D MOC HFG calculation mainly due to underestimated resonance escape probability, i.e., larger attenuation of within-group spectrum, caused by smaller values of fuel-to-moderator ratio in EDCs than in the actual lattice. Figure 3-5 shows the absolute errors of U-238 capture reaction rate per fission neutron. Reaction rate errors are not too big for the cross section errors due to opposite flux errors caused by cross section errors, resulting in moderate range of reaction rate errors. For the homogenized compact problem, 1.87 and 1.93 more neutrons out of 10^5 fission neutrons per fuel pin are captured by U-238 on average in the UFG/2D MOC HFG scheme and the UFG/EDC HFG scheme, respectively; they are very similar, resulting in only a few pcm eigenvalue differences between them. For the heterogeneous compact problem, 0.288 more and 0.0769 less neutrons out of 10^5 fission neutrons per fuel pin are captured by U-238 on average in the UFG/2D MOC HFG scheme and the UFG/EDC HFG scheme, respectively. Similar trends on U-238 capture rate errors are observed for the B₄C rodged case, but the eigenvalue differences between the UFG/2D MOC HFG scheme and the UFG/EDC HFG scheme mainly come from the capture rate difference in the B₄C region.

RMS (root mean square) and maximum values of pin power errors are within an acceptable level as shown in Table 3-1. Figure 3-6 shows the pin power distribution of Serpent2 and relative errors of MC²-3 for the B₄C rodged case. MC²-3 pin powers are slightly flatter than Serpent2, but to a very small extent of $\sim 0.5\%$ at maximum.

Figure 3-4. U-238 Capture Cross Section Errors of MC²-3 Compared to Serpent2 at Four Pins (3, 9, 14 and 16 in Figure 3-2) for the B₄C Unrodded Case.

Figure 3-5. U-238 Capture Reaction Rate Errors per Fission Neutron of MC²-3 Compared to Serpent2 at Four Pins (3, 9, 14 and 16 in Figure 3-2) for the B₄C Unrodded Case.

Figure 3-6. Pin Power Distribution Results of Serpent2 and Relative Errors of MC²-3 for Homogeneous and Heterogeneous Compact Problems of the B₄C Rodded Case.

4. Code Verification for SFR Benchmarks

4.1 Background

The MC²-3 code has been widely used to generate multigroup cross sections for various fast reactor problems, producing solutions in good agreement with Monte Carlo solutions within 200-300 pcm in eigenvalue for most cases. Recently, it was reported [8,9] that MC²-3/DIF3D calculations for an SFR problem resulted in large differences in eigenvalue from Monte Carlo solutions when using simplified computational options. Therefore, the SFR benchmark cases were devised and investigated to figure out what could cause such large differences and whether BG cross sections were generated properly for the core.

4.2 Fuel Assembly Cross Section Generation

Multigroup cross sections for a heterogeneous geometry assembly should be generated, accounting for the heterogeneity effect. The best way is to generate cross sections using the actual geometry. MC²-3 is able to directly solve a 2D assembly problem using the method of characteristics (MOC) which however takes long to generate cross sections. Therefore, a 1D calculation using CPM is preferred to generate cross sections for a heterogeneous geometry assembly. In this case, the first thing to consider is how to construct a 1D model which should be made similar or equivalent to the 2D assembly model.

Among two types of fuel assembly models shown in Figure 4-1, for a fuel assembly without duct, a pin cell (e.g., 3 rings with fuel, cladding, and coolant regions) with an adjusted volume of coolant preserving the total volume ratio of coolant in the assembly can be selected as a representative 1D model.

Figure 4-1. 2D Fuel Assembly Models with or without Duct

Figure 4-2. 1D Fuel Assembly Models

For a fuel assembly with duct, a 1D model may be constructed based on a pin cell with additional regions (i.e., 5 rings with fuel, cladding, coolant, duct, and coolant regions - see Figure 4-2 (c)) or an increased volume of cladding (i.e., 3 rings with fuel, cladding, and coolant regions - see Figure 4-2 (b)) when cladding and duct materials are the same. However, it was observed that 3-ring or 5-ring models cannot represent a 2D assembly geometry with duct accurately because these models do not account for the impact of a duct to resonance self-shielding of fuel pins at different locations.

Control assembly cross sections are generated with a 1D multi-region geometry, similar to the way of generating fuel assembly (FA) cross sections. However, since there is no fissionable material in a control assembly, a large-size additional ring should be added to an outside ring with a FA composition or a mixed core composition excluding control assemblies, as shown in Figure 4-3. Then, for resulting BG cross sections, only control assembly regions are homogenized and condensed using the input option available in MC²-3.

The use of homogenized control assemblies in a core calculation overpredicts the control rod worth due to the neglected spatial self-shielding effect. The overpredicted control worth effect may not be significant in a fast reactor system, compared to a thermal reactor system, because of a longer mean free path of fast neutrons, but the remaining error would not be negligible. Therefore, a cross section correction such as an assembly discontinuity factor (ADF) may be needed in future to improve the accuracy of control rod worth if errors are noticeable. As a control assembly geometry is normally symmetric, it would not be difficult to apply ADFs to cross sections without changing DIF3D.

In this study, note that the cross section generation for a heterogeneous geometry control assembly was not investigated, just using the homogenized control assemblies in the test core and focusing on the cross section generation for a heterogeneous geometry FA.

Figure 4-3. Control Assembly Model

4.3 Benchmark Core Calculations

The reference core of this study is a full-core 3D geometry of a SFR core at the beginning of a cycle (BOC) which was modeled by both Serpent2 and DIF3D. For simplicity, the BOC compositions of all FAs and axial regions were averaged into two compositions corresponding to the “inner zone” (fuel rings 2–4) and the “outer zone” (fuel rings 5–6). Figure 4-4 depicts the core model used in this work.

In this study, the benchmark core was selected to test the cross section generation process using MC²-3/TWODANT. The compositions of the problem are similar to the original core design which was simplified for the test such that only FAs keep a heterogeneous geometry structure and all non-fuel regions including reflector, shield, and control assemblies are homogenized. For simplicity, the core boundary is formed by the outmost shield assemblies in the benchmark core as well. There was no additional approximations made to axial configurations.

As shown in Figure 4-4, the benchmark core is composed of 11 hexagonal assembly rings with 313 assemblies which include 30 inner FAs, 36 outer FAs, 10 test assemblies, 9 control assemblies, 114 reflector assemblies, and 114 shield assemblies.

Figure 4-4. Overview of the SFR Benchmark Core

4.3.1 Assembly Problems

Fuel cross sections were generated using the multi-region cylindrical model with 37 rings, preserving volumes of each material: fuel, cladding, coolant, and duct. Table 4-1 shows the comparison of eigenvalues for the inner FA. The MC²-3 eigenvalue of the homogeneous material agreed very well with the Serpent2 solution within 13 pcm, indicating that resonance self-shielding was accurately conducted in MC²-3.

For the heterogeneous FA, as discussed in the previous section, it was noticed that while the MC²-3 eigenvalues for the 3-region and 5-region cylindrical models have large differences of ~220 pcm Δk from the Serpent2 solution, eigenvalues for the multi-region model (shown in Figure 4-2 (a)) were in good agreement with the Serpent2 solution. As a result, the heterogeneity effects of the FA are 378 pcm Δk from Serpent2 and 380 pcm Δk from MC²-3 with the multi-region model, which are in very good agreement each other. It was noticed that the MOC calculation in MC²-3 with the exact 2D geometry resulted in a good eigenvalue solution but a bit larger difference compared to the multi-region result for this case. As discussed in the previous section, a CPM calculation for a multi-region problem runs much faster than a MOC calculation for a 2D assembly problem in MC²-3.

To see the effect of duct in terms of cylindrical models, additional calculations were conducted for a FA without duct, in which the duct was replaced by coolant. As shown in Table 4-1, if there is no duct, a 3 or 5-region model is sufficient to accurately generate cross sections accounting for the 1D effect.

The cross sections of non-FAs were generated using the two-step approach described in the previous section: i.e., the first step with UFG cross section generation using MC²-3 and then an R-Z core calculation using TWODANT, and the second step with BG cross section generation using MC²-3 and region-wise solutions obtained from TWODANT.

Table 4-1. Eigenvalue Comparison of Inner Fuel Assemblies with or without Duct

Configuration	Serpent2 (k_{∞})	MC ² -3	
		Condition	Δk , pcm
Homogeneous FA	1.68702 $\pm$ 6	Homogeneous	-13
Heterogeneous FA w/ Duct	1.69080 $\pm$ 7	3-region 1D	-221
		5-region 1D	-223
		Multi-region 1D	-11
		2D (MOC)	-71
Heterogeneous FA w/o Duct	1.73120 $\pm$ 6	3-region 1D	-42
		5-region 1D	-31

Since non-FAs are all homogeneous in this study, it is straightforward to generate cross sections for them. In the first step, the 1041-group macroscopic cross section were generated using MC²-3, which were used for an R-Z core calculation using TWODANT. In the second step, 33-group cross sections were generated by condensing UFG cross sections using the region-wise flux and moment solutions obtained from the TWODANT R-Z calculation. All cross sections were generated using ENDF/B-VII.0 data at the temperature of 300K.

One of the important things in the two-step calculations is to make an R-Z model consistent with the SFR benchmark core since the final solution from DIF3D using BG cross sections generated from TWODANT is noticeably affected by what R-Z model is used. A detailed investigation on the effect of an R-Z model will be discussed in the later section.

4.3.2 2D Core Problems

For systematic studies, a 2D model (see Figure 4-5 (a)) was constructed based on the fuel layer (128.100 cm - 212.334 cm high from the bottom) of the 3D problem. The 2D model was further simplified by removing test (except for the test assembly at the core center) and control rod assemblies to minimize approximations when converting the 2D model to a 1D cylindrical model for a TWODANT calculation. Figure 4-5 (b) shows the final 2D model that was used for the study, which was converted to a 1D cylindrical model preserving volumes of each material region, which is composed of a test assembly, inner FAs, outer FAs, reflector assemblies and shield assemblies.

Thirty-three group cross sections were generated using the two-step procedure with MC²-3/TWODANT. Fuel cross sections cross sections were also generated using Serpent2/GenISOTXS

[16] for comparison. For more systematic comparison, two 2D models with homogeneous or heterogeneous FAs were tested. Non-FAs are homogeneous for both models.

Figure 4-5. 2D Benchmark Cores Based on the Fuel Layer of the 3D Benchmark Core

For heterogeneous FAs, a multi-region (or multi-ring) cylindrical model was used to generate 33-group cross sections, as discussed in the previous section. The inner and outer FAs include 3.56 wt.% and 3.48 wt.% U-235 enriched fuel pins, respectively. Both fuel pins have 2.21 wt.% Pu total, but the fuel pin in the outer FA includes ~20% more fission products than that in the inner FA.

A 1D cylindrical model with 5 regions (test, inner fuel, outer fuel, reflector, and shield assembly regions) was developed preserving volumes of each material region in the 2D hexagonal model. A TWODANT calculation was performed with a SN order of S_{12} and an anisotropic scattering order of P_5 .

While testing TWODANT 1D models for BG cross section generation, it was noticed that DIF3D solutions with 33-group cross sections were noticeably affected by a 1D cylindrical model used for TWODANT. The simplified 2D model tested here could be easily converted to a 1D model with minor approximation, but it is difficult to avoid severe approximations in making a 1D model when the actual 2D model includes test and control assemblies located in the middle of hexagonal rings, as shown in Figure 4-5 (a).

DIF3D 2D calculations were conducted with the 6th order source, 6th order flux, and 1st order leakage spatial approximations, varying an angular order from P3 to P9 and an anisotropic scattering order from P1 to P5.

Table 4-2 lists eigenvalues resulted from Serpent2 and DIF3D for the two 2D models: one with homogeneous FAs and the other with heterogeneous FAs. For brevity, these models are denoted as homogenous FA and heterogenous FA, respectively. DIF3D eigenvalues were almost converged with P5P3 (an angular order of P5 and anisotropic scattering order of P3). As shown in the table,

DIF3D eigenvalues with P9P3 agreed well with Serpent2 by -140 pcm and -57 pcm for the core models with homogeneous assemblies or heterogeneous assemblies, respectively. Note that self-shielding cross sections above the resonance energy range were not applied to the cross sections for the 2D core models, which would increase DIF3D eigenvalues by ~50 pcm and accordingly reduce the differences from Serpent2 by that much.

On the other hand, cross sections were generated from Serpent2 and tested in DIF3D calculations to examine their performance. DIF3D calculations were conducted with the P5P3 option only. Since non-fuel cross sections generated from Serpent2 caused large errors, only fuel cross sections generated from Serpent2 were used for the core calculations together with non-fuel cross sections obtained from MC²-3. As shown in Table 4-3, DIF3D eigenvalues with the mixed cross sections generated from Serpent2 and MC²-3 resulted in 120 pcm and 156 pcm differences from Serpent2 for the 2D cores with homogeneous FA or heterogeneous FA, respectively.

Further investigation on cross sections generated from Serpent2 indicated that the reflector cross sections are sources causing the large eigenvalue difference. However, reasons for the poor reflector cross sections were not investigated in this study.

The heterogeneity effect of FAs in the 2D core is 389 pcm from Serpent2, 471 pcm or 425 pcm from DIF3D with MC²-3 cross sections or DIF3D with the mixed cross sections produced from MC²-3 (non-FAs) and Serpent2 (FAs), respectively. The heterogeneity effect was overestimated in DIF3D with MC²-3 cross sections by ~82 pcm, compared to Serpent2. However, when using the mixed cross sections, DIF3D overestimated it by ~36 pcm.

In order to eliminate any ambiguity or approximation arising from group collapsing, 1041-group cross sections were directly used for DIF3D calculations, which does not require the two-step process including a TWODANT calculation with an R-Z model. As seen in Table 4-4, DIF3D solutions agreed well with Serpent2 within ~100 pcm more consistently, resulting in very good agreement in the heterogeneity effect within 22 pcm. This indicates that MC²-3 UFG cross sections themselves are accurate, the differences shown in Table 4-2 are caused by group collapsing with R-Z solutions, and therefore selecting an R-Z model as well as group collapsing need to be made carefully to keep the accuracy.

For detailed investigation, BG macroscopic total cross sections were compared between Serpent2 and MC²-3, revealing that they are in very good agreement with each other for all regions except for those of fuel composition in the low energy range below 20 eV in which neutron fluxes are very small and accordingly their contributions to core eigenvalue and reaction rates are insignificant. It is interesting to note that the macroscopic total cross sections of reflector are in good agreement between Serpent2 and MC²-3 as well, but the use of the reflector cross sections generated from Serpent2 resulted in a large error, which implies that there must be some problems in higher order terms of scattering cross sections.

Table 4-2. Eigenvalue Comparison of the 2D Benchmark Core (the Simplified Model) Solutions with MC²-3 33-group Cross Sections

Configuration	Serpent2 (k_{eff}) $\pm\sigma$ pcm	DIF3D	
		Order	Δk , pcm
Homogeneous FA	1.34931 ± 7	P3P1	-215
		P5P1	-205
		P7P1	-204
		P9P1	-201
		P5P3	-147
		P7P3	-144
		P9P3	-140
		P5P5	-147
		P7P5	-144
		P9P5	-140
Heterogeneous FA	1.35321 ± 7	P3P1	-132
		P5P1	-122
		P7P1	-121
		P9P1	-119
		P5P3	-65
		P7P3	-62
		P9P3	-58
		P5P5	-65
		P7P5	-62
		P9P5	-57
Heterogeneity effect, pcm	389	P5P3	471

Table 4-3. Eigenvalue Comparison of the 2D Benchmark Core (the Simplified Model) Solutions with 33-group Cross Sections Generated from Serpent2 (FAs) and MC²-3 (non-FAs)

Configuration	Serpent2 (k_{eff}) $\pm\sigma$ pcm	DIF3D P5P3 (Δk , pcm)		
		MC ² -3 XS	Serpent2 XS	
Homogeneous FA	1.34931 ± 7	-147	Fuel only	120
			Fuel+Test+Shield only	143
			All including reflector	1359
Heterogeneous FA	1.35321 ± 7	-65	Fuel only	156
Heterogeneity effect, pcm	389	471		425

Table 4-4. Eigenvalue Comparison of the 2D Benchmark Core (the Simplified Model) Solutions with 1041-group Cross Sections

Configuration	Serpent2 (k_{eff}), $\pm\sigma$ pcm	DIF3D P5P3 (Δk , pcm)
Homogeneous FA	1.34931 ± 7	107
Heterogeneous FA	1.35321 ± 7	85
Heterogeneity effect, pcm	389	367

The test results for the 2D core models indicated are summarized as follows:

- DIF3D solutions with 1041-group cross sections were in very good agreement with Serpent2 solutions within 107 pcm. The heterogeneity effects from MC²-3/DIF3D and Serpent2 calculations agreed well with each other.
- DIF3D solutions with 33-group cross sections were influenced by an R-Z model used for a TWODANT calculation whose region-wise flux and moment solutions are used to condense UFG to 33-group cross sections.
- DIF3D solutions were almost converged with P5P3.
- DIF3D solutions with 33-group cross sections generated from MC²-3 agreed well with Serpent2 solutions within 150 pcm.
- DIF3D solutions with 33-group cross sections generated from Serpent2 (FAs) and MC²-3 (non-FAs) agreed well with Serpent2 solutions within ~150 pcm as well. The reflector cross sections generated from Serpent2 caused large errors in DIF3D calculations due to higher order moments of scattering cross sections.

4.3.3 3D Core Problems

The BG cross sections for the 3D benchmark core were generated in the same manner as those for the 2D core, except for an R-Z model which was made represent the 3D core as closely as possible. Fuel assembly cross sections with heterogeneous geometry were generated by calculating a 1D multi-region cylindrical geometry problem, which accounts for a local heterogeneity in the cross section. To consider the region-wise spectrum effect of the core for group condensation, TWODANT solutions for an R-Z model were input to MC²-3 to condense UFG to BG (33 groups) cross sections. The important thing in the fuel cross section generation is that both the local heterogeneity and region-wise spectrum effects should be accounted for together by conducting a 1D multi-region calculation along with an R-Z UFG solutions obtained from TWODANT.

To see the impact of R-Z models, two R-Z models were created for tests: the first model (named as RZ-1, shown in Figure 4-6) with 11 radial and 12 axial regions and the second model (named as RZ-2, shown in Figure 4-7) with 15 radial and 12 axial regions. The former model was created by just selecting one or the majority when there is more than one assembly type in an assembly ring (e.g., rings with test, control, and fuel assemblies together), while the latter model was formed by including all assembly types with preserved volumes. The latter model is considered as more accurate.

Figure 4-6. R-Z Model with 11 Radial and 12 Axial Regions (RZ-1)

Figure 4-7. R-Z Model with 16 Radial and 12 Axial Regions (RZ-2)

Additionally, self-shielded cross sections above the resonance energy range may be needed for more accurate solutions, which is relevant to intermediate-weight isotopes including Fe, Cr, Ni, etc. Those cross sections are not resonance cross sections and thus are not affected by temperature changes. Note that the PENDF cross section library is required for MC²-3 to self-shield those cross sections.

Using the 33-group cross sections generated in the way discussed in the previous section, DIF3D calculations were performed for the 3D benchmark core which is composed of homogeneous non-FAs and heterogeneous FAs. Additional calculations were conducted for the same 3D benchmark core with homogeneous FAs as well in order to check the accuracy of the cross section generation approach for the simpler case with less approximations involved.

Serpent2 calculations were performed to provide reference solutions for comparison. The number of neutron particle histories were chosen to keep a standard deviation of eigenvalue below 10-15 pcm. The unresolved resonance option was turned on and the ENDF/B-VII.0 data at the temperature of 300K (identified with suffix .70c) provided by LANL were used to minimize any errors arising from differences in Doppler broadening between raw data sets. Serpent2 was used for cross section generation as well to compare BG cross sections in detail and see the effect of using those cross sections for core calculations.

In DIF3D, the transport approximation order was changed from P3 to P5, and the anisotropic scattering order was progressed from P1 to P3, ending up with P5P3 (P5 transport approximation and P3 anisotropic scattering approximation).

Table 4-5 shows the results from DIF3D with the 33-group cross sections generated without using TWODANT R-Z solutions. As expected, DIF3D P5P3 solutions with homogeneous or heterogeneous FAs produced as large differences as 921 pcm or 633 pcm from the corresponding Serpent2 solutions, respectively.

Table 4-6 lists the eigenvalues for the 3D benchmark cores, which were produced from Serpent2 and DIF3D P5P3 calculations with 33-group cross sections generated with TWODANT R-Z solutions, showing very good agreement between the two codes within 112 pcm (71 pcm for the case with heterogeneous FAs). Note that the 33-group cross sections generated using TWODANT R-Z solutions were used in the DIF3D calculations. According to the results from progressed transport and anisotropic scattering orders, the effect of the transport approximation order of P5 against P3 is ~130 pcm, and the effect of the anisotropic scattering approximation order of P3 against P1 is ~150 pcm, indicating that the eigenvalue solution even with P5P3 may not be converged yet, unlike the test results with the 2D core.

Using the RZ-1 model for group collapsing, the eigenvalue estimation by DIF3D looks improved for the case with homogeneous FAs but more underestimated for the case with heterogeneous FAs. The choice of R-Z models changed DIF3D eigenvalues by up to 130 pcm, indicating that the impact of an R-Z model is noticeable and an R-Z model should be determined carefully when generating BG cross sections.

The heterogeneity effect of the 3D core is 601 pcm from Serpent2 but 429 pcm from DIF3D, which are different by 172 pcm. Based on the fact that the heterogeneity effect of the FAs is estimated well compared to the Serpent2 solution (see Table 4-1) and the eigenvalue of the 3D core with homogeneous assemblies agreed well with the Serpent2 solution (see Table 4-6), the relatively poor estimation of the heterogeneity effect of the 3D core with heterogeneous FAs may be attributed to the accuracy loss in the BG cross sections of FAs prepared for the 3D core. A further study is needed to pinpoint sources of the accuracy loss and figure out resolutions.

Table 4-5. Eigenvalue Comparison of the 3D Benchmark Core Solutions with MC²-3 33-group Cross Sections Using No R-Z Models

Configuration	Serpent2 (k_{eff}) $\pm\sigma$ pcm	DIF3D	
		Order	Δk , pcm
Homogeneous FA	1.03359 $\pm$ 12	P3P1	-1291
		P5P1	-1156
		P5P3	-921
Heterogeneous FA	1.03960 $\pm$ 12	P3P1	-930
		P5P1	-796
		P5P3	-633
Het. Effect, pcm	601	P5P3	889

Table 4-6. Eigenvalue Comparison of the 3D Benchmark Core Solutions with MC²-3 33-group Cross Sections Using R-Z Models

Configuration	Serpent2 (k_{eff}) $\pm\sigma$ pcm	DIF3D (Δk , pcm)				
		Order	RZ-1		RZ-2	
			w/o SS above Res.	w/ SS above Res.	w/o SS above Res.	w/ SS above Res.
Homogeneous FA	1.03359 $\pm$ 12	P3P1	-370	-303	-228	-162
		P5P1	-236	-169	-99	-31
		P5P3	-75	-16	53	112
Heterogeneous FA	1.03960 $\pm$ 12	P3P1	-540	-494	-402	-346
		P5P1	-402	-359	-270	-214
		P5P3	-240	-202	-119	-71
Het. Effect, pcm	601	P5P3	436	415	429	418

* RZ-1: R-Z model with large approximations, RZ-2: R-Z model with relatively small approximations

For detailed investigation of cross sections, 33-group cross sections for FAs were generated from Serpent2 for the 3D core model, which were used in DIF3D for the 3D core calculation. As discussed in the 2D benchmark core, the MC²-3 generated cross sections were kept for non-FA

cross sections since those cross sections generated from Serpent2 made DIF3D solutions far off from the Serpent2 solutions.

As seen in Table 4-7, DIF3D eigenvalues with the mixed cross sections from Serpent2 and MC²-3 were in very good agreement with the Serpent2 solutions within 45 pcm and 334 pcm for the 3D cores when the non-FA cross sections were generated from MC²-3 with the RZ-1 or RZ-2 model, respectively. It was also noticed that the magnitude of differences for the cases are consistent regardless of FA geometries, resulting in the heterogeneity effect that agreed very well with Serpent2.

Table 4-7. Eigenvalue Comparison of the 3D Benchmark Core Solutions with 33-group Cross Sections Generated from Serpent2 (FAs) and MC²-3 (non-FAs)

Configuration	Serpent2 (k_{eff})	DIF3D P5P3	
		R-Z Model for non-FAs	Δk , pcm
Homogeneous FA	1.03359 ± 12	RZ-1	44
Heterogeneous FA	1.03960 ± 12		45
Het. Effect, pcm	601		602
Homogeneous FA	1.03359 ± 12	RZ-2	332
Heterogeneous FA	1.03960 ± 12		334
Het. Effect, pcm	601		603

* RZ-1: R-Z model with large approximations, RZ-2: R-Z model with relatively small approximations

The fuel and reflector assembly cross sections generated using MC²-3 with or without TWODANT calculation are compared with those from Serpent2 tallies. As shown in Figure 4-8 and Figure 4-9, the TWODANT whole-core calculation accounts for the region-to-region spectral transitions properly and the resulting region-wise spectra significantly reduce the large differences in the cross sections observed in the relatively low energy range below ~2 keV when the TWODANT calculation step was not used. As shown in Figure 4-10, the reflector assembly cross sections are in very good agreement between Serpent2 and MC²-3/TWODANT even in the energy range above the resonance energy of intermediate-weight isotopes (around 1 MeV).

Figure 4-8. Macroscopic Total Cross Sections of Homogeneous Fuel Assembly

Figure 4-9. Macroscopic Total Cross Sections of Heterogeneous Fuel Assembly

Figure 4-10. Macroscopic Total Cross Sections of Reflector Assembly with Self-shielding Cross Sections above the Resonance Energy Range

5. Conclusions

Three tasks and updates associated with MC²-3 were discussed in this report: 1) a MC²-3 library generation using the ETOE-2 code for ENDF/B-VII.1 and ENDF/B-VIII.0 data, 2) a performance improvement in resonance self-shielding for a two-dimensional (2D) assembly calculation using the method of characteristics (MOC) for cross section generation, and 3) an analysis on the correct procedure of accurately generating broad-group cross sections for a sodium-cooled faster reactor (SFR) problem.

First, attempts were made to generate cross section libraries using ENDF/B-VII.1 and ENDF/B-VIII.0 data. Processing ENDF/B-VIII.0 data for the MC²-3 library was more challenging than ENDF/B-VII.1 data because of an increased number of isotopes and different formats and data in many isotopes. We overall successfully generated the ENDF/B-VII.1 MC²-3 library, conducting preliminary verification tests using the selected fast reactor benchmark problems. However, processing the ENDF/B-VIII.0 data was not completed due to many issues encountered in generating MC²-3 libraries using ETOE-2 and running MC²-3 with the processed libraries. Even though the initial work demonstrated the successful generation of the MC²-3 libraries for some isotopes, substantial efforts should be spent to complete processing all 556 isotopes in ENDF/B-VIII.0 data. The lessons learned from processing and verifying the ENDF/B-VII.1 and ENDF/B-VIII.0 libraries of MC²-3 suggested that significant efforts would be required for thoroughly verifying the ENDF/B-VII.1 MC²-3 library and successfully processing the ENDF/B-VIII.0 MC²-3 library. Therefore, further work will continue in future to complete processing the ENDF/B-VIII.0 MC²-3 library and perform more detailed and thorough V&V for the ENDF/B-VII.1 and VIII.0 MC²-3 libraries.

Second, we have updated the MC²-3 code to improve the performance of multi-dimensional calculation capability using MOC for cross section generation. In the improved process, the unit-cell problem is first solved to obtain the UFG weighting spectrum which is used to condense UFG to intermediate group cross sections that the lattice calculation using MOC employs. Since the self-shielding calculation based on the MOC fixed-source calculations in a 2D heterogeneous geometry was very expensive, the equivalent Dancoff-factor cell (EDC) method is introduced, which allows the code to solve a 2D assembly fixed-source problem much faster by solving multiple decoupled 1D slowing-down problems. This effort was made useful in implementing and verifying the EDC method in the Griffin cross section API.

Third, we analyzed a SFR problem by generating multigroup cross sections with MC²-3 and performing core calculations with DIF3D in order to investigate reasons for large eigenvalue deviations reported in the conference papers [8,9]. For the analysis, a set of BG cross sections were generated using the spatial calculational models of MC²-3. DIF3D core calculations were performed with these cross section sets, whose results were compared with Monte Carlo solutions. The analysis results demonstrated that all the solutions from MC²-3/DIF3D were satisfactory, being in good agreement with Monte Carlo solutions within 119 pcm in core eigenvalue. This indicated that the large differences reported in the conference papers were attributed to BG cross sections

generated inaccurately. This report provides the correct process of accurately generating broad-group cross sections with MC²-3.

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Nuclear Science and Engineering Division

Argonne National Laboratory
9700 South Cass Avenue, Bldg. 208
Argonne, IL 60439-4842

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