Group Constants Generation using MCS Monte Carlo Code for Fast Reactor Analysis

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1. Introduction

Recently, the homogenized group constant (GC) generation using the continuous-energy Monte Carlo (MC) method for fast reactor analysis has achieved a growing attraction among nuclear reactor physics community. Its motivation is based on the advance of MC method on the simulation of complex reactor geometries without introducing any approximation, which is conventional to the deterministic codes. Therefore, this study aims to present a brief methodology for GC generation by the in-house UNIST MC code MCS [1], that can be compatibly utilized in the nodal diffusion code, RAST-K (R2) [2], to analyze the core behavior of fast reactor. The capability of this approach is quantified on the $3600 MW_{th}$ sodium fast reactor (SFR) oxide core (MOX-3600) from the OECD/NEA SFR benchmark [3]. The solutions of the beginning-of-cycle (BOC) steady-state calculation of MCS/R2 for a wholecore problem, including the core multiplication factor, power profiles, control rod worth (CRW), fuel temperature coefficient (FTC) and coolant temperature coefficient (CTC), are generated and verified with those from the MCS MC code.

2. Computer Codes

Two computer codes are used in this work. One is the UNIST in-house MC code MCS, that is recently featured with GC generation capability. Another is the nodal diffusion code RAST-K for analyzing the fast reactor using the generated GCs by MCS.

MCS is a 3D continuous-energy neutron-physics code for particle transport based on the MC method, under development at UNIST since 2013 [1]. MCS can conduct criticality runs for reactivity calculations and fixed source runs for shielding problems. MCS has been designed from scratch since 2013 to conduct whole-core criticality simulation with pin-wise depletion and thermal/hydraulic feedback. MCS neutron transport capability is verified and validated against several benchmark problems, including the BEAVRS benchmark, ~300 cases from the International Criticality Safety Benchmark Experimental Problem (ICSBEP) and OECD/NEA SRF benchmark.

The RAST-K code has been developed at UNIST for diffusion core calculations [2]. It adopts the 3D nodal method with multi-group (MG) coarse mesh finite difference (CMFD) acceleration technique to solve steady state and transient problems with assembly-level nodes. Recently, the triangular polynomial expansion nodal (TPEN) method has been implemented in RAST-K for fast reactor analysis.

3. Group Constant Generation by MC Method

To tally several targeted GCs, the average neutron flux for a certain geometrical region and for the number of energy ranges (energy group) is initially scored by the MC code [4]:

$$\phi_g = \frac{1}{V} \int_V \mathrm{d}V \int_{E_g}^{E_{g-1}} \mathrm{d}E\phi(r, E) \tag{1}$$

where $\phi(r,E)$ is the space-energy dependent flux, V is the volume and g is the group index with the given energy boundary of E_g .

The certain reaction rates can be tallied by the product of the estimated flux and an interest cross-section (XS):

$$R_{x,g} = \frac{1}{V} \int_{V} dV \int_{E_g}^{E_{g-1}} dE \Sigma_x(r, E) \phi(r, E)$$
(2)

Division of these two integral quantities gives the GC or multi-group cross-section (MG XS) for a specific reaction type x and energy group g:

$$\Sigma_{x,g} = \frac{R_{x,g}}{\phi_g} \tag{3}$$

As mentioned, the generated GCs are to be utilized in nodal diffusion code. The required XSs are therefore total, absorption, the fission and fission production, fission spectrum, transport XS and scattering matrix. It is noted that the weighting function to tally the Pn scattering matrix in this study is simply the scalar energy dependent flux:

$$\Sigma_{s,g \to g'}^{l} = \frac{\frac{1}{V} \int_{V} dV \int_{E_{s}}^{E_{s-1}} dE \int_{E_{s}}^{L} dE' \int_{-1}^{1} d\mu \Sigma_{s} (r, E \to E', \mu) \phi(r, E) P_{l}(\mu)}{\phi_{g}}$$
(4)

where *l* is scattering order, that is also the *l*th order Legendre polynomial coefficient, $P_l(\mu)$, and μ is the cosine angle between incident neutron at *E* and the outgoing neutron at *E*'. The outer-scatter approximation is then applied to tally the transport XS:

$$\Sigma_{tr,g} = \Sigma_{t,g} - \sum_{g'=1}^{G} \Sigma_{s,g \to g'}^{l}$$
(5)

where G is the total number of groups.

4. Solution of the MOX-3600 Whole-core Problem

To quantify the accuracy of the GCs generated by MCS, a large mixed oxide fuel $3600MW_{th}$ SFR (MOX-3600) specified in the OECD/NEA benchmark [3] is

selected for analysis, and its radial quarter core loading pattern is shown in Fig. 1. The core is composed of 225 inner and 228 outer MOX fuel sub-assemblies (SAs) depended on the Plutonium content. Each fuel SA contains 271 helium bonded fuel rods with Oxide Dispersion Strengthened (ODS) steel cladding and enclosed by a hexagonal EM10 steel duct. The fuel rod is divided into 5 axial zones, namely lower gas plenum, lower reflector, fuel, upper gas plenum, and upper reflector as described in Fig. 2a. The radial pattern of the fuel SA is illustrated in Fig. 2b. The surrounding of the core includes 330 radial reflector sub-assemblies. MOX-3000 adopts two reactivity control system, including 24 control SAs as primary control system and 9 control SA as the secondary control system. More detail descriptions are provided in the OECD/NEA benchmark report [3].



Fig. 1. Radial quarter core layout of MOX-3600.



Fig. 2. Description of the fuel sub-assembly: (a) axial zones layout and (b) radial layout.

A set of GCs for each fuel SA is generated using a single 2D model of a fuel SA with reflective boundary conditions, as in Fig. 2b. All homogenized GCs for non-multiplying regions are generated using 2D super-cell models as shown in Fig. 3 [5]. To approximate the flux

that those regions experienced in the core, they are located at the center of the model and surrounded by fuel SA. Furthermore, the super homogenization (SPH) method [5] is applied to correct the flux-volume weighted GC of the strong absorber region and its surrounding region, namely control SA and its surrounding fuel SAs. Nevertheless, the detail method is not to be presented in this paper, the use of the SPH factor in this work is to better estimate the CRW and power profile as rodded condition.

The GC set for 24-group energy structure [5] is obtained by MCS and converted into a compatible database for the nodal diffusion code R2 to simulate a whole-core problem to predict several parameters of interest, including core k_{eff} , radial and axial power profiles, and reactivity feedback coefficients. The energy structure is listed in Tables I. The ENDF/B-VII.0 library is used, where the fuel and other material temperature is set 900K and 600K, respectively. The reference solutions are computed with MC code MCS with the criticality set as follows: 5 inactive batches, 20 active batches, 200 cycles per batch and 20,000 histories per cycle.



Fig. 3. 2D super-cell models for non-multiplying regions.

Table I: 24-group Energy Structure

No.	Upper E (MeV)	Lower E (MeV)
1	1.96403E+01	1.00000E+01
2	1.00000E+01	6.06531E+00
3	6.06531E+00	3.67879E+00
4	3.67879E+00	2.23130E+00
5	2.23130E+00	1.35335E+00
6	1.35335E+00	8.20850E-01
7	8.20850E-01	4.97871E-01
8	4.97871E-01	3.01974E-01
9	3.01974E-01	1.83156E-01
10	1.83156E-01	1.11090E-01
11	1.11090E-01	6.73795E-02
12	6.73795E-02	4.08677E-02
13	4.08677E-02	2.47875E-02
14	2.47875E-02	1.50344E-02
15	1.50344E-02	9.11882E-03
16	9.11882E-03	5.53084E-03
17	5.53084E-03	3.35463E-03
18	3.35463E-03	2.03468E-03
19	2.03468E-03	1.23410E-03
20	1.23410E-03	7.48518E-04
21	7.48518E-04	4.53999E-04
22	4.53999E-04	3.04325E-04
23	3.04325E-04	1.48625E-04
24	1.48625E-04	1.00001E-11

The k_{eff} for 3D core calculation at BOC all rod out (ARO) by MCS/R2 and MCS is summarized in Table II. The radial assembly-wise power distributions at ARO and all rod in (ARI) state by MCS/R2 and MCS are shown in Figs. 4-5. Fig. 6 illustrates the axial power distribution and the comparison between MCS/R2 and MCS. The maximum standard deviation (SD) of MCS radial power at ARO and ARI state is corresponding to 1.27% and 1.85%. It is clearly seen that a great agreement is achieved since the difference in k_{eff} is less than 110 pcm, the root-mean-square (RMS) in power error is less than 0.6% at ARO and less than 1.5% at ARI and the maximum difference in axial power is less than 2.4%. Furthermore, solutions of reactivity feedback coefficients, including CRW, FTC and CTC, are shown in Table II. It is noted that the SPH factor is applied to accurately calculate the CRW. Overall, reactivity feedback coefficients predicted by MCS/R2 are also well agreed with those of MC code MCS since the CRW difference is less than 0.6% and the differences in FTC and CTC are in three MCS's SD.

Table II: MOX-3600 core parameters calculated with MCS and MCS/R2.

Parameter	MCS (±3σ)	MCS/R2	Diff. (±3σ %)
k _{eff}	1.01747 ± 0.00014	1.01856	0.107 ± 0.010
CRW (pcm)	5948±16	5989	0.6±0.3
FTC (pcm/K)	-0.867±0.039	-0.894	3.1±4.5
CTC (pcm/K)	$0.437 {\pm} 0.038$	0.418	-4.5±8.6



Fig. 4. Assembly power distribution at ARO state, MCS/R2 vs. MCS.



Fig. 5. Assembly power distribution at ARI state, MCS/R2 vs. MCS.



Fig. 6. Axial power distribution, MCS/R2 vs. MCS.

5. Conclusions

In this work, the feasibility of utilizing the MCS MC code for generating GCs for fast spectrum 3D simulation with the R2 simulators is investigated. The performance of steady-state analysis with R2 using the 24-group GC data generated by MCS is conducted to predict the core $k_{\rm eff}$, power profiles and reactivity coefficients. A code-tocode comparison shows a great consistency between MCS/R2 and MCS, since the k_{eff} bias is less than 110 pcm, and RMS power difference is less than 0.5% and 1.5% at ARO and ARI state, respectively. The outcome of this study proves the MCS can be a promising tool for GC generation for fast reactor analysis. The future work is focused on the application of MCS for temperature dependent and coolant density dependent GCs for burnup calculation coupled with thermal-hydraulics feedback for fast reactor analysis.

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