Multi-objective Optimization Approach of Multi-Group Cross Section Library for Lattice Transport Code using Non-dominated Sorting Genetic Algorithm-II

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1. Introduction

Various studies have been conducted to develop a high-accuracy multi-group cross section (MGXS) library to improve the accuracy of deterministic multi-group transport analyses. Although many outstanding methods have been discussed, the library generation approach that employs resonance treatment using background cross sections and reference spectra to produce self-shielded group cross sections is the most widely adopted in core design practice in Republic of Korea. [1-2] The Korea Atomic Energy Research Institute (KAERI) has developed its own library generation system based on this approach, and its performance has been validated in many studies. [1, 3-4]

To further enhance prediction fidelity, Kyung Hee University conducted library correction research that modifies lattice code cross sections to follow reference Monte Carlo (MC) reaction rates. [4-5] For automated library optimization, the previous study verified that a heuristic-based library optimization approach can solve diverse benchmark problems with high accuracy. [6]

However, that work was limited to a single objective focused on zero-burnup initial state reactivity error. Practical core analyses must also consider burnup behavior and core power distribution. Accordingly, this study extends the heuristic library optimization framework from a single-objective to a multi-objective and adopts a Non-dominated Sorting Genetic Algorithm II (NSGA-II) to search Pareto fronts over three objectives. [7]

The target benchmark is a LEU+ soluble boron-free (SBF) small modular reactor (SMR) with enrichments ranging from 4.0 to 8.2 w/o. Under varied enrichment and coolant conditions, NSGA-II searches Pareto-optimal solutions across the three objectives and derives corrected MGXS libraries. McCARD [8] is used as the reference MC code, and DeCART2D [9] is used for deterministic multi-group transport analysis.

2. Methods

2.1 Library Correction and Optimization

This study uses the library correction system that can iteratively update the lattice code cross sections using correction factors derived from reaction rate ratio between the lattice code and the reference MC code. [5] For library optimization, the following *library correction options* must be specified:

a. Correction reference model
b. Round-wise target nuclide
c. Nuclide-wise target cross section type
d. Cross section-wise target temperature point

Accordingly, library optimization can be conducted by modifying the library through appropriate combinations of these *correction options* and by searching for the combination that yields the most accurate analysis of the target benchmark. The heuristic algorithm varies correction options *a–d*, evaluates library performance and searches for a global optimum through iterative loops. In the previous study, conventional genetic algorithms (GA) and simulated annealing (SA) were applied. [6, 10-11]

2.2 Multi-object Optimization using NSGA-II

The introduction noted that a lattice transport code must produce accurate results for zero-burnup initial state reactivity, depletion behavior, and core power distribution. Accordingly, this study employs the multi-objective optimization algorithm NSGA-II [7] for library optimization instead of conventional single-fitness heuristic methods.

NSGA-II evaluates individuals encoded as combinations of library correction options and, using fast non-dominated sorting, classifies them into Pareto-ranked fronts. The rank 0 front contains non-dominated solutions, meaning that no solution in this set is simultaneously inferior to another across all objectives. Elitism preserves higher-ranked solutions for the next generation, while crowding distance promotes a well-spread distribution within a front. Offspring are generated from the Pareto set through crossover and mutation.

$$D_n^x = \frac{f_{n+1}^x - f_{n-1}^x}{f_{max}^x - f_{min}^x}. \tag{1}$$

$$D^x = \sum D_n^x . \tag{2}$$

The crowding distance for single objective axis in Eq. (1) is a normalized distances to neighboring solutions. The crowding distance of a single individual shown in

Eq. (2) is the sum of the crowding distances of all objective axes. D denotes the crowding distance, x denotes the objective function type, and n denotes the index of the individual sorted by Pareto dominance. Larger crowding distances indicate less crowded regions in the front, and thus the corresponding individual is preferentially selected within the same rank. Figure 1 presents the flowchart of the library optimization using NSGA-II in this study.

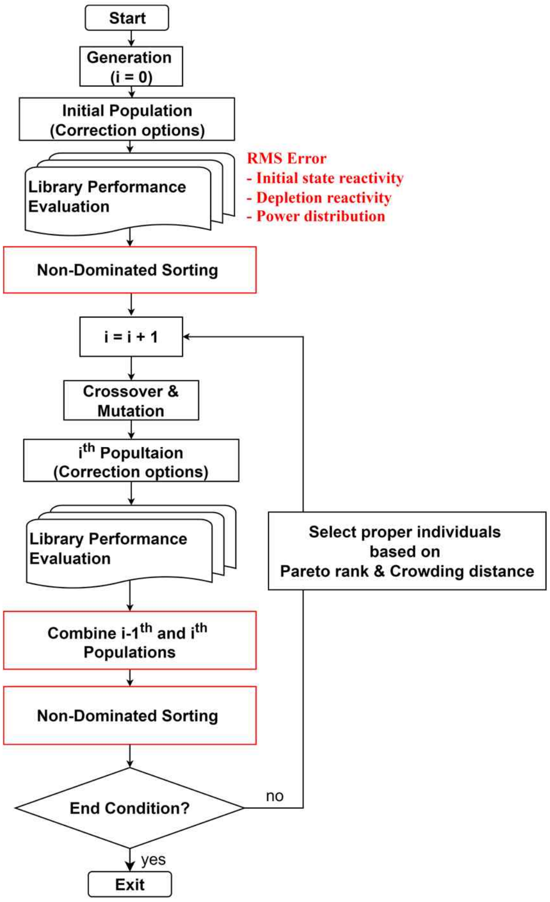

Fig. 1. Flowchart of cross section library optimization using NSGA-II

The objective functions of this study are the weighted averages of RMS errors for initial state, depletion, and power distribution problems, and these can be calculated using weights assigned to each benchmark problem group, as shown in Eq. (3).

$$f^x = \frac{\sum \omega_i RMS_{x,i}}{\sum \omega_i},$$
$$where\ , x \in \{\text{INIT}, \text{DEP}, \text{POW}\}. \tag{3}$$

f^x denotes the objective function subdivided into benchmark problem types; INIT (zero-burnup initial state), DEP (depletion), and POW (power distribution). The ω denotes the benchmark group-wise weight and i indicates the group number. Weights can be assigned according to the importance of each benchmark problem group.

3. Preliminary Optimization for LEU+ SBF SMR Benchmark

This section describes the preliminary optimization of a library for LEU+ SBF SMR design using NSGA-II. The reference MC code McCARD is calculated based on ENDF/B VII.1 version library. The statistical uncertainty of multiplication factor is about 10 pcm for INIT and POW problems, and 30 pcm for the DEP problem.

3.1 Considered SMR Benchmark

The considered benchmark is an LEU+ SMR problems [12] using fuel enrichments from 4.0 w/o to 8.2 w/o. Excess reactivity is controlled by high content gadolinia BA, and stainless steel (SS304) is used as the reflector. Figures 2 and Table II illustrate the configurations of the LEU+ SMR 2D core and fuel assemblies. The benchmark set consists of 15 single-assembly problems defined by five assembly types and three temperature conditions. Additionally, it includes one 2D core problem and one depletion problem burned up to 80 MWd/kgHM using an assembly with an 8.0 w/o enriched UO_2 pin. Table I shows the description of the LEU+ SMR benchmark problems.

Table I. Conditions of LEU+ benchmark problem

Benchmark group	Condition			Temp ID
	T_Fuel [K]	T_Clad [K]	T_Mod [K]	
2D assembly (INIT, 15 problems)	900.0 600.0 300.0	600.0 600.0 300.0	600.0 600.0 300.0	HFP HZP CZP
2D assembly (DEP, 1 problem)	873.15	613.15	577.15	
2D core (INIT, POW, 1 problem)	873.15	613.15	577.15	

* Abbreviation: HFP, HZP, and CZP indicate Hot Full Power, Hot Zero Power, and Cold Zero Power temperature conditions. “Temp ID” is an identification index based on temperature conditions.

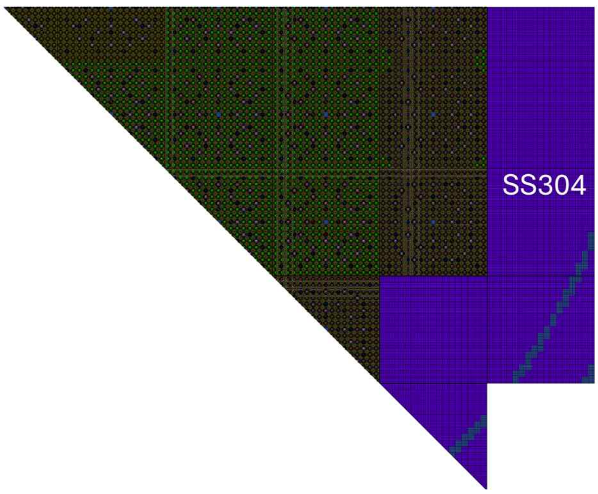

Fig. 2. Configuration of LEU+ 2D core

Table II. Configuration of LEU+ fuel assemblies

Assembly Type	Configuration	Note
W40	4.0 w/o main fuel No BA pin	
W55	5.5 w/o main fuel 32 BA pins	
W80	8.0 w/o main fuel 48 BA pins	5.5 w/o zoned fuel
W81	4.0 w/o main fuel 48 BA pins	
W82	4.0 w/o main fuel 48 BA pins	

* Abbreviation: BA indicates "Burnable Absorber"

The fuel assemblies used in this study are called as W40, W55, W80, W81, and W82 according to the their main UO_2 pins. For example, the W81 uses 8.1 w/o enrichment fuel mainly for its configuration. The W40 assembly is a blanket assembly that is not containing burnable poison rods. Other assemblies are designed with high content gadolinia pins arranged with varying weight fractions. The W80 assembly contains zoned fuel with an enrichment of 5.5 w/o. As previously mentioned, the W80 assembly serves as the target problem for the DEP benchmark in this study.

3.2 NSGA-II library optimization results

A total of 30 generations were executed for the preliminary library optimization. Each generation consisted of a population of 10, and each individual encoded correction options for 5 correction rounds for 3 nuclide groups. The correction target nuclide groups are uranium (^{235}U, ^{238}U), gadolinium (^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, ^{160}Gd), and hydrogen (^{1}H).

All benchmark problem groups are assigned a weight of 1.0. This means that the calculation results from all fifteen 2D assembly problems and a single result from the 2D core problem have the same effect on evaluating the MGXS library performance. The weighting of each benchmark problem group can be varied depending on the importance of the problem.

NSGA-II starts from an uncorrected library in which no nuclide is corrected. Since the uncorrected library was generated without specific consideration for the LEU+ SMR benchmark system, it will exhibit significantly large initial reactivity errors. Although this uncorrected library is not usually used in reactor design practice, it is employed to ensure a fair initial starting point for the NSGA-II optimization. Tables III through V present representative optimization results for three objectives after 30 generations of NSGA-II optimization.

Table III. LEU+ benchmark results at initial generation

Ind*	Weighted RMS Error			Pareto Rank
	INIT* [pcm]	DEP* [pcm]	POW* [%]	
1	656	554	0.62	0
2	656	554	0.62	0
3	656	554	0.62	0
4	656	554	0.62	0
5	656	554	0.62	0
6	656	554	0.62	0
7	656	554	0.62	0
8	656	554	0.62	0
9	656	554	0.62	0
10	656	554	0.62	0

* Abbreviation: Ind indicates "Individual". INIT, DEP, and POW indicate initial state, depletion, and core power distribution categories, respectively.

Table IV. LEU+ benchmark results at 2nd generation

Ind*	Weighted RMS Error			Pareto Rank
	INIT [pcm]	DEP [pcm]	POW [%]	
1	163	218	0.50	0
2	72	188	0.76	0
3	127	107	0.71	0
4	101	190	0.56	0
5	656	554	0.62	1
6	656	554	0.62	1
7	656	554	0.62	1
8	656	554	0.62	1
9	656	554	0.62	1
10	119	218	0.72	1

Table V. LEU+ benchmark results at 30th generation

Ind*	Weighted RMS Error			Pareto Rank
	INIT [pcm]	DEP [pcm]	POW [%]	
1	92	258	0.46	0
2	76	259	0.46	0
3	79	77	0.52	0
4	47	247	0.55	0
5	132	218	0.48	0
6	61	117	0.78	0
7	110	203	0.48	0
8	61	117	0.78	0
9	56	118	0.57	0
10	58	121	0.57	0

In the initial generation, the weighted RMS errors were 656 pcm for INIT, 554 pcm for DEP, and 0.62% for POW problems. In the 2nd generation, a non-dominated solution set improving all three objectives was observed. At the 30th generation, various improved trade-off solutions were obtained at population.

In the final generation, an appropriate solution can be selected from among various trade-offs. For instance, the 4th individual yielded the most accurate result for the INIT benchmark. The 3rd individual showed the highest accuracy for the DEP benchmark, and the 2nd individual (or the 1st) is most optimized for the POW benchmark. However, it was observed that the 2nd and 4th individuals exhibited significant errors in the DEP benchmark results. Therefore, the 3rd individual can be selected as the most balanced solution in this study.

For power distribution, the RMS error sensitivity to library correction is about 0.2%, and slight improvements were observed for evolved individuals. Since nuclide-wise correction factors are applied identically to the same materials within the 2D core, the normalized power distribution is analyzed as having low sensitivity to correction.

Figures 3 through 5 present the LEU+ SMR benchmark results from the initial generation and representative individuals from the final generation for the INIT, DEP, and POW categories.

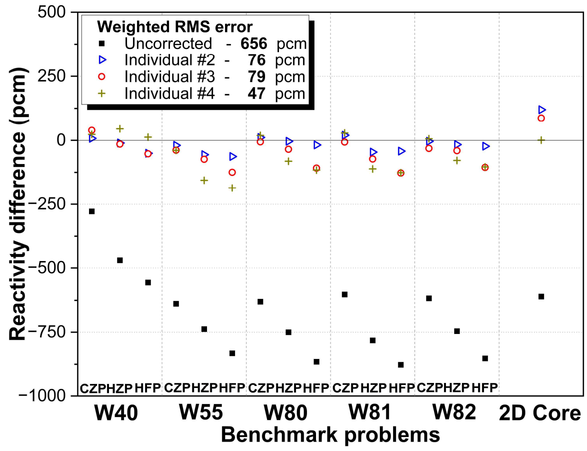

Fig. 3. NSGA-II results for representative individuals at generation 30 for the LEU+ SMR benchmark, zero-burnup initial state reactivity difference (INIT).

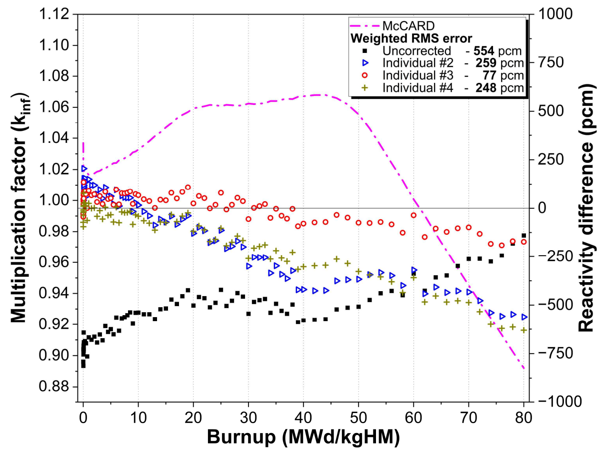

Fig. 4. NSGA-II optimization results of representative individuals at 30th generation for LEU+ SMR benchmark, depletion reactivity difference (DEP)

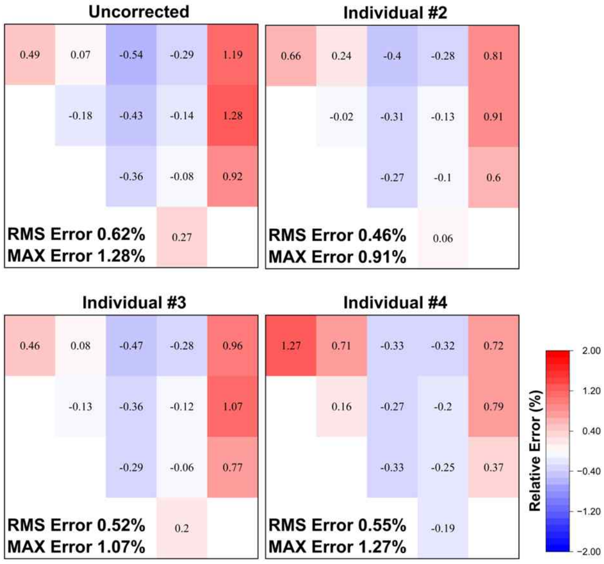

Fig. 5. NSGA-II optimization results of representative individuals at 30th generation for LEU+ SMR benchmark, power distribution (POW)

4. Conclusions

This study presents a strategy for multi-objective optimization of a MGXS library based on the NSGA-II algorithm. The proposed algorithm produced improved non-dominated solution sets over 30 generations with respect to zero-burnup initial state reactivity, depletion behavior, and power distribution, and it demonstrated that the three objectives were optimized to reasonable levels. This NSGA-II–based optimization approach is expected to be applicable to optimize the various MGXS library corrections.

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