Diffusion Analysis of Cylindrical Molten Salt Fast Reactor based on Simplified Few-group GET

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1. Introduction

The Molten Salt Reactor (MSR) [1], classified under the Generation IV International Forum (GIF), boasts distinctive features such as low-pressure operation, utilization of liquid fuel, robust accident resistance, and enhanced fuel utilization efficiency. Addressing the limitations of conventional thermal spectrum-based MSRs, prior research has suggested the implementation of the Molten Chloride Salt Fast Reactor [2] as a potential solution.

Previous research [3][4][5] highlights a substantial variance of several hundred pcm in the reactivity calculation of the Molten Salt Fast Reactor (MSFR) when comparing outcomes derived from the neutron diffusion equation (referred to as NDE) and those obtained using the Monte Carlo method.

This underscores the potential for significant errors in the reactivity calculation of the MSFR when relying solely on a general diffusion theory. Furthermore, research [4][5] indicates that incorporating the discontinuity factor [6] (hereinafter, DF) within nodal equivalence theory proves effective in mitigating reactivity errors. However, previous studies have necessitated full-core Monte Carlo calculations for obtaining accurate reaction cross-sections, which is impractical. In this study, we investigate the applicability of employing cross-sections derived from simplified models, constituting a practical approach.

2. Methods and Results

2.1 Reactor Model

Figure 1 illustrates the reactor model examined in this study, featuring a reflector encompassing the entire reactor core. (Gray: Fuel, Yellow: Side reflector, Orange: Top/bottom reflector).

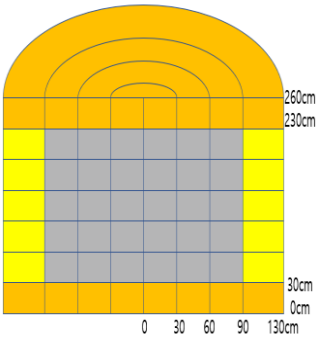

Fig. 1. Molten Salt Fast Reactor Model

The reactor fuel consists of 46KCl-54UCl_3 (enriched to 19.75 wt% U-235 and 99 at% Cl-37), with SS304 serving as the reflector material. Further detailed information about the reactor in this study can be found elsewhere [7].

2.2 Calculation Method

2.2.1 Derivation of Reaction Cross-Sections

In previous studies, nuclear reaction cross-sections for NDE calculations were obtained from full-core models using the SERPENT2 code. This requires a substantial amount of computational resources. Furthermore, full-core Monte Carlo simulations dilute the practical purpose of this study, as it aims to obtaining a reference solution. Therefore, this study aims to utilize nuclear reaction cross-sections derived from simplified models (e.g., infinite cylinder, infinite plane) employed in obtaining the DF for NDE calculations.

In this study, the SERPENT2 code was utilized to generate reference data, encompassing the multiplication factor (k_{eff}), few-group cross-sections, and surface current. Comprehensive details regarding the calculation settings for the SERPENT2 code are provided in Table I.

Table I. Monte Carlo code Information

Code name	SERPENT 2.2.0
Libraries	ENDF/B-VII.1
Particles	500,000
Cycle	Inactive: 200, active: 300

Figures 2 and 3 depict the infinite cylinder model and infinite plane model, respectively. The radial DF is computed using the infinite cylinder model shown in Figure 2, and the reaction cross-sections of both the fuel and radial reflector, utilized in this process, are also applied to the NDE calculation.

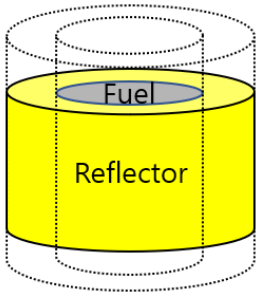

Fig. 2. Infinite Cylinder Model for Radial DF

Similarly, the axial DF is computed using the infinite plane model shown in Figure 3, and the reaction cross-sections of the top and bottom side reflector, utilized in this process, are applied to the NDE calculation.

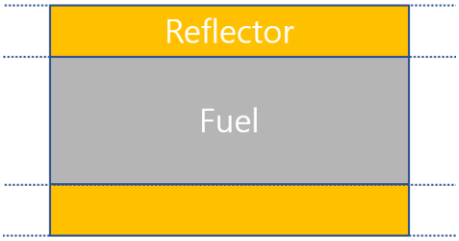

Fig. 3. Infinite Plate Model for Axial DF

2.2.2 NDE Calculation

Due to the broad energy spectrum of fission reactions in fast reactors, it is essential to categorize them into multiple energy groups, where in total of 9 energy groups are considered in this study as below:

Table II. Energy Groups

Group	Upper Bound Energy (MeV)
1	20
2	6.07
3	1.35
4	4.98E-01
5	1.83E-01
6	6.74E-02
7	2.48E-02
8	9.12E-03
9	3.35E-03

The MSFR fuel is treated as a homogenized mixture, implying homogeneous reaction cross-sections of fuel throughout the medium. The Finite Difference Method (FDM) is used in this study to solve NDE. The node size for the FDM was determined to achieve sufficiently converged values for the NDE calculation, with convergence reached at a node size of 2.5 cm.

3. Results

3.1 Initial Core

The results of the initial core analysis using cross-sections derived from simplified models were compared with those obtained using cross-sections obtained from the full-core model. Additionally, these results were compared with reference values obtained from the SERPENT2 code.

Table III compares the reaction cross-sections of the nuclear fuel obtained from the simplified model with those obtained from the full-core simulation. As seen in Table III, the reaction cross-sections of the nuclear fuel obtained from the simplified model are similar to those obtained from the full-core model.

Table III. Comparison of the differences in the reaction cross-sections of the initial core.

Group	Σ_{tr}	Σ_a	Σ_f	$\nu\Sigma_f$
1	0.01%	-0.04%	0.02%	0.02%
2	0.02%	-0.13%	-0.07%	-0.10%
3	-0.03%	-0.06%	-0.09%	-0.10%
4	-0.03%	0.05%	0.04%	0.04%
5	-0.09%	0.08%	0.05%	0.04%
6	-0.23%	0.10%	0.06%	0.06%
7	-0.19%	-0.15%	-0.12%	-0.12%
8	-0.42%	-0.60%	-0.80%	-0.80%
9	-0.32%	-1.10%	-0.98%	-0.98%

Table IV presents a comparison of the derived cross-sections applied to the NDE calculation in each case. The results were compared with reference values obtained from the SERPENT2 code. Notably, there is no significant discrepancy observed in the NDE calculation, even when utilizing cross-sections derived from simplified models used for the DF calculation.

Table IV. Result of Initial Core

Method		k_{eff}	Difference [pcm]
SERPENT2 (Reference)		1.01343 ±0.00005	0.0
Full-core model	w/o DF	1.02520	1132.9
	w/ DF	1.01324	-18.5
Simplified model	w/o DF	1.02500	1113.8
	w/ DF	1.01310	-32.1

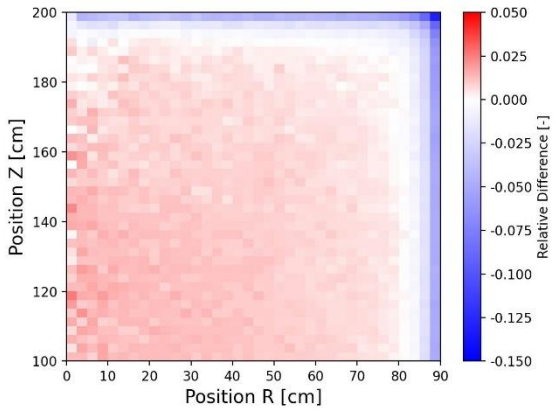

Fig. 4. Relative error of power density in the initial core

Figure 4 compares the power distribution of the SERPENT2 code with that of the case where reaction cross-sections derived from the simplified model and DF are applied. In total, the core has a root mean square error of 1.5%. The corners where the reflector interfaces exhibit a noticeable error of -13.0%.

3.2 Burned Core

To analyze the burned core, identifying depleted materials is necessary. This study assumes a 10-year

depletion period, focusing solely on nuclear fuel. Unlike the previous approach [7], where cross-sections are obtained from the depletion of the full-core model, burnup calculation using the simplified infinite cylinder model has been considered in this study.

Comparing burned fuel compositions from full-core and infinite cylinder models exhibits noticeably similar results. The comparison focuses on the atomic fraction of the top 40 nuclides, encompassing 99% of the total. The method for generating the DF remains consistent, utilizing burned fuel composition from the infinite cylinder model and applying nuclear reaction cross-sections to the NDE, analogous to the approach used for the initial core.

The results from a 10-year burned core analysis using simplified models were compared with the full-core model. While the full-core model involved depletion and cross-section calculations within the full-core model, Table V contrasts fuel reaction cross-sections from the simplified model with those from the full-core model. Despite performing depletion and reaction cross-section calculations in the infinite cylinder model for the simplified approach, there is no significant difference observed compared to values from the full-core model.

Table V. Comparison of the differences in the reaction cross-sections of the 10y Burned core.

Group	Σ_{tr}	Σ_a	Σ_f	$\nu\Sigma_f$
1	-0.01%	-0.04%	0.07%	0.10%
2	0.07%	-0.04%	0.04%	0.06%
3	0.05%	0.14%	0.18%	0.26%
4	0.07%	0.23%	0.27%	0.36%
5	0.01%	0.21%	0.19%	0.27%
6	-0.13%	0.21%	0.10%	0.19%
7	-0.06%	0.03%	-0.08%	0.01%
8	-0.31%	-0.27%	-0.58%	-0.49%
9	-0.52%	-2.36%	-2.53%	-2.48%

Table VI compares the application of the obtained cross-sections to the NDE calculations, referencing values from the SERPENT2 code. In the full-core model, the initial over-a-thousand pcm error diminishes to just a few pcm, attributed to comprehensive burnup and cross-section calculations within the full core. Conversely, the simplified model exhibits a slight increase in the difference. Nevertheless, even in this case, the improvement effect remains substantial compared to scenarios without applying the DF.

Table VI. Result of Initial Core

Method		k_{eff}	Difference [pcm]
SERPENT2 (Reference)		0.84939 ±0.00005	0.0
Full-core model	w/o DF	0.85753	1117.6
	w/ DF	0.84932	-9.7
Simplified model	w/o DF	0.85833	1226.2
	w/ DF	0.85024	117.7

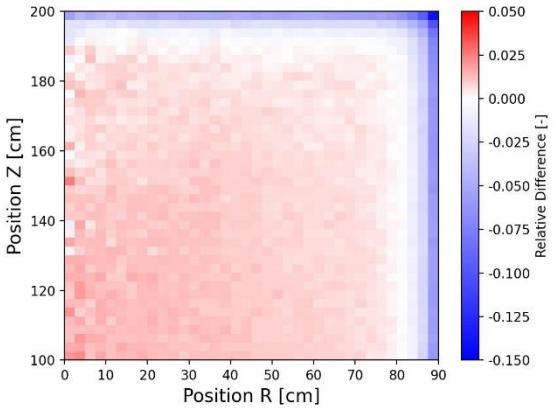

Fig. 5. Relative error of power density in the burned core

Figure 5 compares the power distribution obtained from the SERPENT2 code with that obtained when utilizing reaction cross-sections derived from the simplified model and DF. The core displays a 1.7% root mean square error, with a substantial -14.0% error observed at the corners near the reflector interfaces.

3.3 Enhancing Power Density Distribution in Corner Regions

The Simplified GET method has demonstrated a significant improvement in the accuracy of k_{eff}. However, as shown in Figures 4 and 5, noticeable errors persist in the power density distribution at the core periphery, particularly where the upper/lower reflectors intersect the side reflector. The few-group cross-sections of the nuclear fuel in this study are assumed homogeneous throughout the core. However, there's a discrepancy between the core-wide cross-sections and those in the corner regions affected by nearby reflectors. Obtaining group cross-sections for the corner region from the full-core model is the most accurate method but not aligned with this study's objective. Hence, a simple bar-shaped model is proposed as a suitable approximation, considering the insensitivity of neutron-weighted cross-sections to calculation structures.

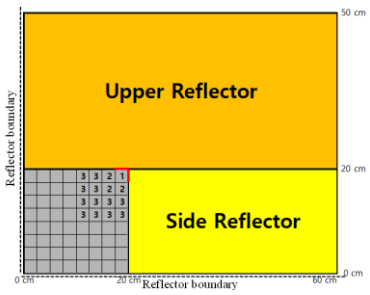

Fig. 6. Cross-sectional view of the simple bar model

Figure 6 illustrates the cross-sectional view of the simplified bar model, which simplifies the toroidal corner region of the MSFR, as shown in Figure 1, into a basic bar shape. It consists of a bar shape with infinite length positioned between an upper reflector and a side

reflector, with nuclear fuel in between. To calculate the group cross-sections for the corner area, the 10cm × 10cm corner region is divided into three segments. The fuel area is doubled to create a marginal area, with reflective boundaries established on the left and bottom sides. Particularly for region 1, where two sides are in contact with the reflectors, the corner DF value for this region was determined separately and applied in the NDE calculations.

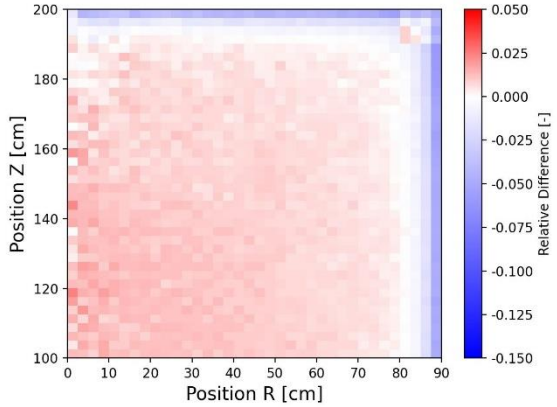

Fig. 7. Improvement in power distribution via corner region cross-sectional application (initial core)

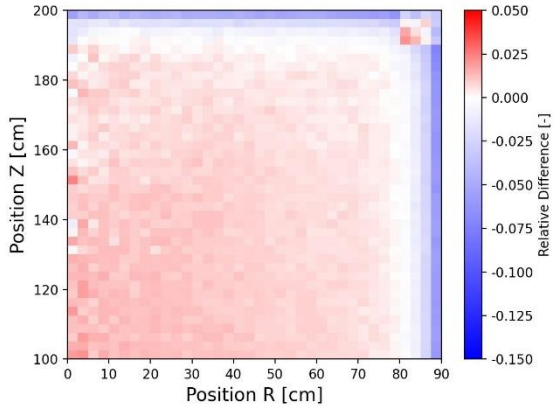

Fig. 8. Improvement in power distribution via corner region cross-sectional application (burned core)

Figures 7 and 8 illustrate how incorporating cross-sectional information from the corner region improves the power density distribution in that area. The results showed a reduction in the error from over 13% to less than 5% in the corner region in both the initial core and the burned core. Therefore, it can be concluded that using simplified simulated corner region cross-sections and DF is effective in reducing the power density error in the corner region.

4. Conclusion

This study investigated the applicability of Simplified GET-based multi-group diffusion theory for the MSFR model. The results suggest that utilizing simplified models for deriving reaction cross-sections and DFs in NDE calculations for MSFR yields promising outcomes. The effective application of simplified diffusion theory is evident in both initial core and burned core analyses, validated against SERPENT2 code reference values. Comparisons with results from full-core Monte Carlo simulations indicate that simplified models offer accurate estimations, particularly with a significant reduction in computational resources.

However, it was observed that the application of DF did not significantly reduce the error in power density distribution. This discrepancy stems from the neglect of multi-group cross-section variations within the nuclear fuel, which vary depending on its location. Particularly, the error in power density distribution at the corner region was notably higher compared to other areas. To address this issue, additional consideration was given to multi-group cross-sections and DF at corner points within the nuclear fuel region. Even with values obtained from a simple bar-shaped geometry model, there was an improvement effect.

Acknowledgments

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※ DAPA: Defense Acquisition Program Administration

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