Proceedings of the Reactor Physics Asia 2023 (RPHA2023) Conference
Gyeongju, Korea, October 24-26, 2023

Burnup-dependent Discontinuity Factors for Diffusion Analysis of Molten Salt Fast Reactors

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1. Introduction

The Molten Salt Reactor (MSR), one of the Generation IV International Forum (GIF) [1] reactor, has several characteristics such as low-pressure operation, liquid fuel, accident resistance and very high fuel utilization, etc. Addressing limitations of conventional MSR designs primarily relying on thermal spectrum, recent research has advocated for the adoption of the Molten Chloride Salt Fast Reactor [2]. Previous investigations [3-4] have exposed a noteworthy divergence, amounting to several hundred pcm, in reactivity calculations for the Molten Salt Fast Reactor (MSFR) when contrasting results obtained from the neutron diffusion equation (referred to herein as NDE) with those from the Monte Carlo method. This emphasizes that depending solely on a general diffusion theory can lead to substantial inaccuracies in computing the reactivity of the MSFR.

Recently, it was discovered that incorporating the discontinuity factor [5] (referred to here as DF) from the nodal equivalence theory could also effectively reduce reactivity errors for MSFR reactors [4]. Additionally, it was recognized that applying the DF calculated for the initial core to the burning core also yields beneficial effects in enhancing reactivity [6]. However, if it were possible to easily obtain DF values based on burnup, the calculations for the reactivity of the burning core would become more accurate. This study aims to propose a method for interpolating and utilizing the DF as a function of fuel burnup.

2. Model and Methods

2.1 Reactor Model

Figure 1 shows a reactor model considered in this study, in which the reflector surrounds the entire reactor core. (Gray: Fuel, Yellow: Side reflector, Orange: Top/bottom reflector). The reactor fuel consists of 46KCl-54UCl_3 (enriched to 19.75 wt% U-235 and 99 at% Cl-37), while the reflector material is stainless steel 304. Further detailed information pertaining to the reactor in this study can be found elsewhere [6].

2.2 Calculation Method

2.2.1 Monte Carlo Method

The SERPENT2 code was used in this study to generate reference data, including multiplication factor

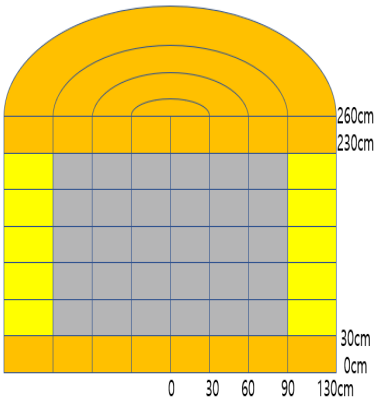

Fig 1. Side, Top/bottom Reflector MSFR

(k_{eff}), group libraries, and surface current. Details of the calculation settings for the SERPENT2 code are presented 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

The reactor depicted in Figure 1 was simulated for a 10-year burnup calculation with a thermal power of 400 MW using the SERPENT2 code. Table II presents k_{eff} values and the inventory of major fuel materials as a function of burnup. The study aims to assess the suitability of NDE methodology, applying equivalence theory, for modeling reactivity changes with burnup for MSFR system. Sub-criticality due to burnup was not considered.

Table II. Burnup Information

Year	Burn-up (MWd/kgU)	k_{eff}	U-235 (kg)	U-238 (kg)	Pu-239 (kg)
0	0.00	1.01344 ± 0.00032	2189.5	8896.0	0.0
2	26.34	0.98142 ± 0.00031	1873.7	8724.8	122.9
4	52.68	0.94860 ± 0.00033	1582.6	8543.1	234.5
6	79.02	0.91491 ± 0.00035	1317.4	8350.1	333.9
8	105.36	0.88188 ± 0.00037	1079.3	8145.3	420.7
10	131.70	0.84882 ± 0.00040	869.2	7928.7	494.6

2.2.2 NDE Method

Since fission reactions occur across a wide energy spectrum in fast reactors, it is necessary to partition them into multiple energy groups. For the neutron diffusion equation (NDE) method in the presented study, 9 energy groups are utilized, and their specifications are outlined in Table III.

The MSFR fuel is treated as being uniformly mixed, implying that the nuclear data remains constant regardless of its position within the fuel. To solve this equation, the Finite Difference Method (FDM) is employed.

Table III. 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

3. Calculation Strategy and Results

3.1 DF values for initial core and burned core

The DF at material interfaces is determined using only two representative values (one for each direction facing the interface) for each energy group. To evaluate the DF for the lateral reactor materials, the SERPENT2 code is applied with an infinite cylinder model. Similarly, an infinite plate model is used to compute the DF at the interface between the fuel and the upper reflector. The FDM grid size used for generating DFs is 10 cm.

Tables IV and V represent the DF values for the initial core, while Tables VI and VII show the DF values for the core after 10 years of burnup. Note that DF values were annotated by adding a "+" or "-" sign to the material names, indicating the DF values for the outer and inner surfaces, respectively. An extra parameter, denoted as α (alpha), is introduced to account for the ratio between the surface flux and the surface current at the vacuum interface, derived from the SERPENT2 result.

Table IV. DF values (Initial core-side)

Group	Fuel+	Reflector-	Reflector+	α
1	9.96662E-01	6.92194E-01	1.75515E+00	1.32489E+00
2	1.03379E+00	7.61744E-01	6.17153E-01	1.48179E+00
3	1.01850E+00	9.96449E-01	1.56233E+00	1.60375E+00
4	1.04730E+00	9.93529E-01	-1.63059E+00	1.64949E+00
5	1.03955E+00	1.08102E+00	-1.09910E+00	1.67296E+00
6	1.00934E+00	1.11302E+00	-5.70333E-01	1.70476E+00
7	1.24580E+00	9.88746E-01	-6.68273E-01	1.72473E+00
8	1.12314E+00	1.96269E+00	-2.21442E-01	1.72344E+00
9	9.25539E-01	1.07904E+00	-4.37433E-01	1.72909E+00

Table V. DF values (Initial core-top/bottom)

Group	Fuel+	Reflector-	Reflector+	α
1	1.00452E+00	7.05944E-01	6.27977E-01	1.35471E+00
2	1.04695E+00	7.71657E-01	5.54631E-01	1.47341E+00
3	1.02448E+00	9.94664E-01	1.19593E+00	1.64848E+00
4	1.05681E+00	9.98831E-01	-1.73653E+01	1.69442E+00
5	1.03934E+00	1.09073E+00	-4.73197E+00	1.70437E+00
6	1.00158E+00	1.13272E+00	-1.33268E+00	1.71626E+00
7	1.28322E+00	1.03033E+00	-1.77705E+00	1.73469E+00
8	1.16065E+00	2.63017E+00	-3.85551E-01	1.74635E+00
9	9.23829E-01	1.30400E+00	-7.55424E-01	1.73281E+00

Table VI. DF values (10y Burned core-side)

Group	Fuel+	Reflector-	Reflector+	α
1	1.00422E+00	6.91235E-01	4.95179E+00	1.31294E+00
2	1.03704E+00	7.59817E-01	6.47940E-01	1.49622E+00
3	1.01738E+00	9.92209E-01	1.60291E+00	1.60307E+00
4	1.04660E+00	9.87586E-01	-1.55607E+00	1.65056E+00
5	1.03826E+00	1.07198E+00	-1.05744E+00	1.67032E+00
6	1.00380E+00	1.09080E+00	-5.59074E-01	1.70119E+00
7	1.22785E+00	9.71546E-01	-6.50896E-01	1.72067E+00
8	1.12093E+00	1.42148E+00	-2.24005E-01	1.72652E+00
9	9.22419E-01	1.36285E+00	-4.89886E-01	1.72735E+00

Table VII. DF values (10y Burned core-top/bottom)

Group	Fuel+	Reflector-	Reflector+	α
1	1.00863E+00	7.09582E-01	7.22647E-01	1.31325E+00
2	1.05194E+00	7.70803E-01	5.62817E-01	1.47772E+00
3	1.02228E+00	9.91571E-01	1.21750E+00	1.64386E+00
4	1.05537E+00	9.92027E-01	-1.14099E+01	1.69364E+00
5	1.03621E+00	1.07886E+00	-4.20193E+00	1.69971E+00
6	9.94823E-01	1.10519E+00	-1.30850E+00	1.71813E+00
7	1.25241E+00	9.99947E-01	-1.70716E+00	1.73865E+00
8	1.14922E+00	1.58558E+00	-4.17345E-01	1.74012E+00
9	9.09721E-01	1.65496E+00	-9.63618E-01	1.72868E+00

3.2 Calculation of DF values as a function of burnup

Using Tables IV and VI, the DF for the lateral side of the core was determined as a function of burnup, and utilizing Tables V and VII, the DF for the top/bottom of the core was determined as a function of burnup. Utilizing the DF values obtained from the initial core and the core after 10 years of burnup, the DF values are expressed as a first-order function with respect to burnup, following Equation 1.

$$DF(X) = \frac{10y\ DF - initial\ DF}{10y\ burnup} X + initial\ DF, \quad (1)$$
$$X\ is\ equal\ to\ burnup$$

Tables VIII and IX present the DF values for the core after 4 years of burnup [52.68 MWd/kgU], calculated using the function described earlier. The α value was also determined from a first-order equation based on burnup, similar to the method used to calculate the DF values.

Table VIII. DF values (4y Burned core-side)

Group	Fuel+	Reflector-	Reflector+	α
1	9.99685E-01	6.91810E-01	3.03381E+00	1.32011E+00
2	1.03509E+00	7.60973E-01	6.29468E-01	1.48756E+00
3	1.01805E+00	9.94753E-01	1.57856E+00	1.60348E+00
4	1.04702E+00	9.91152E-01	-1.60078E+00	1.64992E+00
5	1.03903E+00	1.07740E+00	-1.08244E+00	1.67190E+00
6	1.00712E+00	1.10413E+00	-5.65829E-01	1.70333E+00

7	1.23862E+00	9.81866E-01	-6.61322E-01	1.72311E+00
8	1.12226E+00	1.74621E+00	-2.22467E-01	1.72467E+00
9	9.24291E-01	1.19256E+00	-4.58414E-01	1.72839E+00

Table IX. DF values (4y Burned core-top/bottom)

Group	Fuel+	Reflector-	Reflector+	α
1	1.00616E+00	7.07399E-01	6.65845E-01	1.33813E+00
2	1.04895E+00	7.71315E-01	5.57905E-01	1.47513E+00
3	1.02360E+00	9.93427E-01	1.20456E+00	1.64663E+00
4	1.05623E+00	9.96109E-01	-1.49831E+01	1.69411E+00
5	1.03809E+00	1.08598E+00	-4.51995E+00	1.70251E+00
6	9.98877E-01	1.12171E+00	-1.32301E+00	1.71701E+00
7	1.27090E+00	1.01818E+00	-1.74909E+00	1.73627E+00
8	1.15608E+00	2.21233E+00	-3.98269E-01	1.74386E+00
9	9.18186E-01	1.44438E+00	-8.38702E-01	1.73116E+00

The method of applying the DF to the NDE is outlined through Equations 2 and 3. Equation 2 represents the net current continuity equation at the boundary between the nuclear fuel and the reflector material. Equation 3 represents the relationship between the reflector and vacuum boundary. The FDM grid size used to solve the NDE is the same as the size used for DF generation, which is 10 cm.

$$J_g^{i,i+1} = \frac{2}{\left(\frac{\Delta r_{i+1} f_g^{i+1,-}}{D_g^{i+1}}\right)+\left(\frac{\Delta r_i f_g^{i,+}}{D_g^{i}}\right)}\left(\bar{\phi}_g^i f_g^{i,+} - \bar{\phi}_g^{i+1} f_g^{i+1,-}\right) \quad (2)$$

$$J_g^{N,R} = \frac{D_g^N}{\frac{\Delta r_N}{2}+D_g^N \frac{\alpha}{f_g^{N,R}}}\bar{\phi}_g^N \quad (3)$$

3.3 Result

Table X presents the results of reactivity calculations utilizing the DF values acquired via a burnup-dependent interpolation function for 2, 4, 6, and 8 years.

Table X. Results of the reactivity calculation

Year (MWd/kgU)	Method	k_{eff}	Difference (pcm)
2 year (26.34)	SERPENT2	0.98139 ± 0.00005	0.0
	NDE (without DF)	0.99229	1119.3
	NDE (with DF)	0.98166	28.0
4 year (52.68)	SERPENT2	0.94859 ± 0.00005	0.0
	NDE (without DF)	0.95915	1160.6
	NDE (with DF)	0.94885	28.9
6 year (79.02)	SERPENT2	0.91534 ± 0.00005	0.0
	NDE (without DF)	0.92548	1197.0
	NDE (with DF)	0.91548	16.7
8 year (105.36)	SERPENT2	0.88196 ± 0.00005	0.0
	NDE (without DF)	0.89182	1253.6
	NDE (with DF)	0.88209	16.7

Even without relying on the DF values obtained through the use of an infinite lattice model, using the interpolated DF values obtained from two burnup states still leads to highly accurate calculations of core reactivity for each burnup.

3. Conclusions

As nuclear fuel undergoes burnup, the constituents of the nuclear fuel change, resulting in variations in the composition of the fuel. Consequently, the values of the DF also change accordingly. For an analysis of the burning core, it is necessary to determine the DF values for each specific burnup condition. By utilizing the DF values from two burnup states, it is possible to derive the DF values as a function of burnup through interpolation. As a result, it was possible to accurately calculate reactivity within a range of a few tens of pcm. This approach can help reducing computational effort involved in calculating DF values for individual burnup states.

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