# Full-Core Analysis of Thorium-Fueled Molten Salt Breeder Reactor Using the SERPENT 2 Monte Carlo Code

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## INTRODUCTION

The Molten Salt Reactor (MSR) is an advanced type of reactor which was developed at Oak Ridge National Laboratory (ORNL) in the 1950s and was operated in the 1960s. In the MSR, fluorides of fissile and/or fertile materials (i.e. $UF_4$, $PuF_3$ and/or $ThF_4$) are mixed with carrier salts to form a liquid fuel which is circulated in a loop-type primary circuit [1]. This innovation leads to immediate advantages over traditional, solid-fueled, reactors. These include near-atmospheric pressure in the primary loop, relatively high coolant temperature, outstanding neutron economy, a high level of inherent safety, reduced fuel preprocessing, and the ability to continuously remove fission products and add fissile and/or fertile elements [2].

The thermal spectrum Molten Salt Breeder Reactor (MSBR) was designed to realize the promise of the thorium fuel cycle, which uses of natural thorium instead of enriched uranium. Thorium breeds fissile $^{233}U$ and avoids uranium enrichment. The mixture of LiF-$BeF_2$-$ThF_4$-$UF_4$-$PuF_3$ has a melting point of 499°C, a low vapor pressure at operating temperatures, and good flow and heat transfer properties [3]. The MSBR complex geometry is challenging to describe in software input and usually require major geometric approximations [4].

We used the continuous-energy Serpent 2 Monte Carlo particle transport code to calulate whole-core depletion in the MSBR. We then compare these results with existing MCNP6 results with a more simplified geometric model [4, 5]. This neutronics model is of sufficient fidelity to inform optimization of fuel salt composition, fuel utilization, neutron fluxes, and spectrum evaluation. Moreover, this model will be employed for depeletion calculations, generation of problem-oriented homogenized nuclear data (multi-group cross sections and diffusion constants) for deterministic reactor codes, and multiphysics simulations [6, 7].

All calculations presented in this paper were performed using Serpent 2 version 2.1.28. Serpent 2 levereges hybrid OpenMP + MPI parallelized memory management, which enabled us to conduct depletion calculations on computer clusters with multiple cores [8].

In Section 2, a brief description of the MSBR geometry model is given. In Section 3 the results are presented and discussed. Section 4 reflects conclusions and plans for future research.

## MSBR DESIGN DESCRIPTION

The MSBR vessel has diameter of 680 cm and a height of 610 cm. It contains a molten fluoride fuel-salt mixture that generates heat in the active core region and transports that heat to the primary heat exchanger by way of the primary salt pump. In the active core region, the salt flows through channels in moderating and reflecting graphite blocks.

The core has two radial zones bounded by a solid cylindrical graphite reflector and the vessel wall. Zones I and II are surrounded radially and axially by fuel salt. This space for fuel is necessary for injection and flow of molten salt.

Fig. 1 shows the plan view of the whole-core configuration at the expected reactor operational level when both graphite control rods are fully inserted, and the safety rods are fully withdrawn. The safety rods only get inserted during an accident.

Fig. 2 shows the longitudinal section of the reactor. The violet color represents bare graphite, and the yellow represents fuel salt. The blue color shows Hastelloy-N, a material used for the plenum and vessel wall, and the black color is a void space. In this work, all figures of the core were generated using the built-in Serpent plotter.

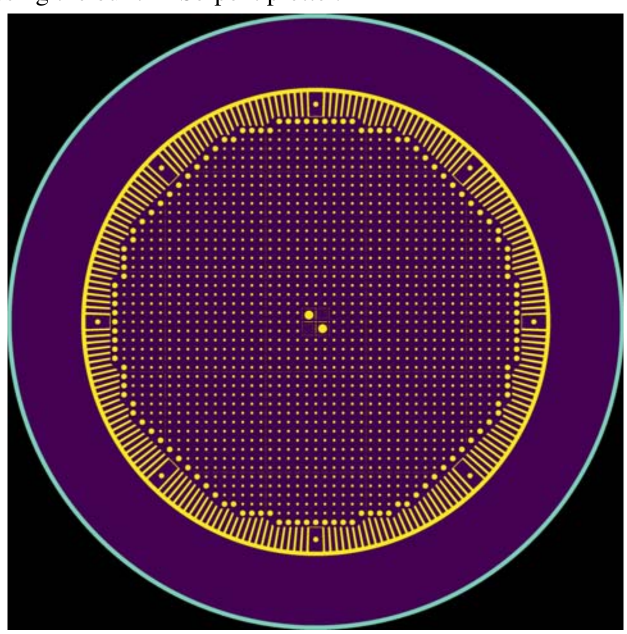

Fig. 1: Plan view of MSBR core.

### Core Zone I

The central portion, called Zone I, is made up of 1320 graphite elements, each 10.16cm×10.16cm×396.24cm. In Zone I, 13% of the volume is fuel salt and 87% is graphite. Zone I is composed of 1320 graphite cells and 4 channels for control rods: two for graphite rods which both regulate and shim during normal operation, and two for backup safety rods to assure sufficient negative reactivity for emergency

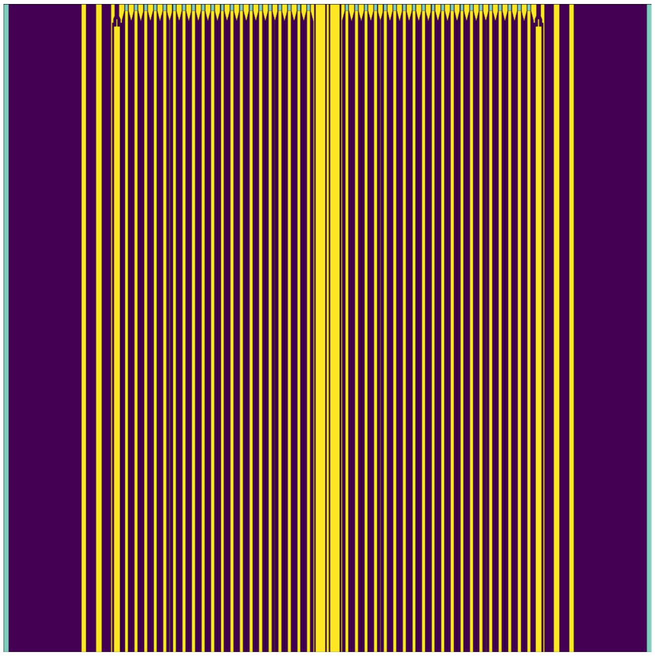

Fig. 2: Elevation view of MSBR core.

situations.

These graphite elements have a mostly rectangular shape with lengthwise ridges at each corner that leave space for salt flow elements. Various element sizes reduce the peak damage flux and power density in the center of the core prevent local graphite damage. Figure 3 demonstrates the elevation and sectional views of graphite elements exactly as they are represented in this Monte Carlo model.

### Core Zone II

The undermoderated zone, Zone II, surrounds Zone I. Combined with the bounding radial reflector, Zone II serves to diminish neutron leakage. This zone is formed of two kinds of elements: elements like those in Zone I with a larger channel diameter (Zone II-A), and radial graphite slats (Zone II-B).

Zone II is Zone II 37% salt by volume and each element has a fuel channel diameter of 6.604cm. It is divided into two different zones: Zone II-A and Zone II-B. The graphite elements for Zone II-A are prismatic. Zone II-B elements are rectangular slats spaced far enough apart to provide the 0.37 fuel salt volume fraction. Fig. 4 additionally shows the 5.08cm-wide annular space between the core graphite and the radial reflector graphite. The annulus contains 100% fuel salt and serves to reduce the damage flux at the internal surface of the graphite reflector blocks. The reactor Zone II-B graphite 5.08cm-thick slats vary in the radial dimension (average width is 26.67cm) but are reconstructed without any approximation. From the ORNL report [3], the suggested design of Zone II-B has 8 irregularly-shaped graphite elements every 45° as well as salt channels. These graphite elements were simplified into right-circular cylindrical shapes with central channels. This is the only simplification made to the MSBR conceptual geometry in this work.

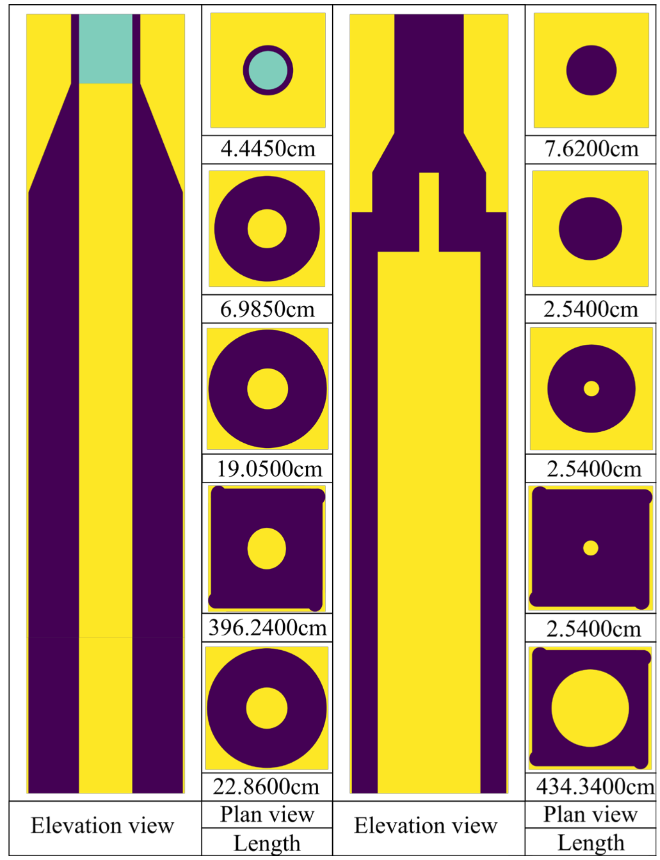


Fig. 3: Zone I (left) and Zone II-A (right) elements.

### Material composition

The fuel salt, the reactor graphite, and the modified HastelloyN are materials unique of the MSBR and were created at ORNL. The initial fuel salt loading composition is LiF-$BeF_2$-$ThF_4$-$^{233}UF_4$ (71.8-16-12-0.2 mole %). The lithium in the molten salt fuel is a fully enriched $^7$Li because $^6$Li is a very strong neutron poison and becomes tritium upon neutron capture. For cross section generation, ENDF/B-VII was employed [9]. The specific temperature was fixed for each material to correctly model the Doppler-broadening of resonance peaks when Serpent generate problem-oriented nuclear data library.

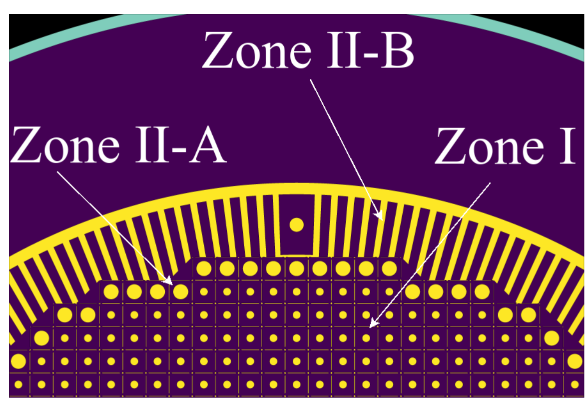


Fig. 4: Plan view that includes Zone I, II-A, and II-B elements.

## RESULTS

This section presents calculation results, such as the effective multiplication factor for whole core, neutron flux spectrum, and temperature reactivity coefficients. The normalized neutron flux distribution is calculated for the whole core using continuous-energy nuclear data. The temperature coefficients for both fuel salt solution and reactor graphite are computed by comparing effective multiplication factors for two temperatures in the working range.

### Neutron spectrum

Fig. 5 demonstrates the normalized neutron flux spectrum for the whole core in the energy range from $10^{-9}$ to 10 MeV. The results show close fit with the MCNP simulation [4], especially in thermal energy range. It is important to obtain the epithermal and thermal spectrum to produce $^{233}$U from $^{232}$Th because radiative capture cross section of thorium monotonically decreases from $10^{-10}$ MeV to $10^{-5}$ MeV. Hardening the spectrum tends to significantly increase resonance absorption in thorium and decrease the absorptions in fissile and construction materials. Thus, a signficant amount fissile material will be needed to make the reactor critical.

### Effective multiplication factor

Table I shows the effective multiplication factor for both MCNP6 and Serpent 2 whole core models. The factor obtained using Serpent 2 is 300 pcm lower than that obtained by Park *et al.* using MCNP6 [4]. Standard deviations are 5 and 9 pcm, respectively. The discrepancy is likely due to simplificiations to the Zone II geometry model used in Park *et al.*

### Temperature effect of reactivity

Table II shows temperature effects on reactivity calculated in this work as compared to both [4] and [3]. Uncertainty for each temperature coefficient also appears in Table II. The main physical principle underlying the reactor temperature feedback is an expansion of matter when it is heated. When the fuel salt temperature increases, the density of the salt decreases, but at the same time, the total volume of fuel salt in the core remains constant because it is bounded by the graphite. When the reactor graphite temperature grows, the density of graphite declines creating additional space for fuel salt. To determine temperature coefficients, the cross-section temperatures for fuel and moderator were changed from 900K to 1200K. Three different cases were considered:

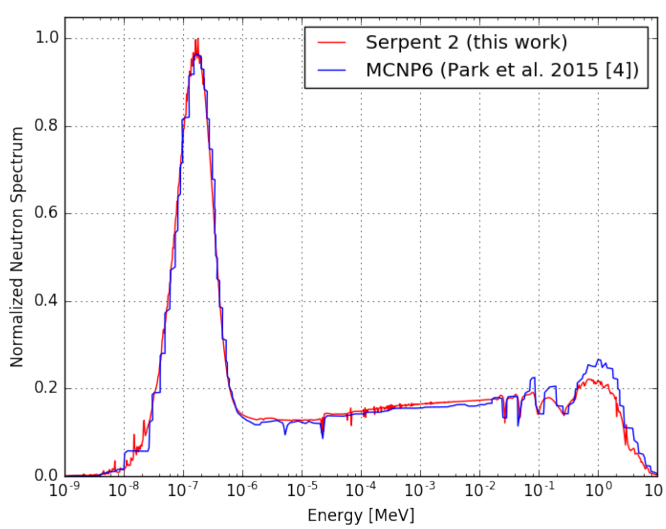


Fig. 5: Neutron flux spectrum of MSBR for MCNP6 and Serpent 2 model.

TABLE I: Effective multiplication factor of whole core model.

| | Serpent2 | MCNP6 [4] |
|---|---|---|
| $K_{eff}$ | 1.00389±0.00005 | 1.00736±0.00009 |

1. Temperature of fuel salt rising from 900K to 1200K.
2. Temperature of graphite rising from 900K to 1200K.
3. Whole reactor temperature rising from 900K to 1200K.

TABLE II: Temperature coefficients of reactivity.

| Reactivity coefficient [pcm/K] | Serpent2 | MCNP6 [4] | Reference [3] |
|---|---|---|---|
| Fuel salt | −3.70 ± 0.016 | −3.20 ± 0.05 | −3.22 |
| Moderator | +2.33 ± 0.027 | −0.11 ± 0.05 | +2.35 |
| Total | −1.57 ± 0.033 | −3.21 ± 0.04 | −0.87 |

In the first case, changes in the fuel temperature only impact fuel density. In this case, the geometry is unchanged because fuel is a liquid. However, when the moderator heats up, both the density and the geometry change due to thermal expansion of the solid graphite blocks and reflector. Accordingly, the new graphite density was calculated using a linear temperature expansion coefficient of $1.3\times10^{-6}$1/K [3]. A new geometry input was created based on this information.

The fuel temperature coefficient (FTC) is negative due to thermal Doppler broadening of the resonance capture cross sections in the thorium and is in a good agreement with early research [3, 4]. The moderator temperature coefficient is positive due to changing density and would increase during reactor operation because of spectrum hardening along with fuel depletion [4]. Finally, the total temperature coefficient of reactivity is relatively large and negative, despite graphite components, and affords excellent reactor stability and controllability.

## CONCLUSIONS

We performed MSBR full-core analysis using the Serpent 2 Monte Carlo code. The complex geometry of the reactor is reconstructed in three-dimensional space without any major approximations. Accurate material data was employed to calculate reactor key design parameters. The effective multiplication factor for initial fuel composition is slightly higher than 1 (1.00389) which allows reactor operation from startup to the first online reprocessing cycle. The neutron flux energy spectrum was calculated for the whole core and represents the epithermal spectrum of the MSBR. The total temperature coefficient is negative, consequently, the MSBR has negative temperature feedback, but MTC is negative which has a negligible effect on safety because it is outweighed by the strong, negative FTC.

This high-fidelity full-core model will be employed for a number of future efforts. First, depletion simulation will be performed using Serpent 2 depletion capabilities to find the equilibrium state of the MSBR, its optimal fuel salt composition, reprocessing characteristics (i.e. rates of removing fission products, the rate of adding thorium), and fuel utilization. Secondly, the model will be used to generate problem-oriented nuclear data libraries for multi-physics models of MSRs developed in the MOOSE-based coupled neutronics/thermal-hydraulics code Moltres [10]. Finally, transient accident simulations for safety investigation of the reactor core will be performed to study the dynamic behavior of Molten Salt Breeder Reactor.

## REFERENCES

1. P. N. HAUBENREICH and J. R. ENGEL, "Experience with the Molten-Salt Reactor Experiment," *Nuclear Technology*, **8**, *2*, 118–136 (Feb. 1970).
2. D. LEBLANC, "Molten salt reactors: A new beginning for an old idea," *Nuclear Engineering and Design*, **240**, *6*, 1644–1656 (Jun. 2010).
3. R. C. ROBERTSON, "Conceptual Design Study of a Single-Fluid Molten-Salt Breeder Reactor." Tech. Rep. ORNL–4541, comp.; Oak Ridge National Lab., Tenn. (Jan. 1971).
4. J. PARK, Y. JEONG, H. C. LEE, and D. LEE, "Whole core analysis of molten salt breeder reactor with online fuel reprocessing: Whole core analysis of MSBR with online fuel reprocessing," *International Journal of Energy Research*, pp. n/a–n/a (Jul. 2015).
5. J. LEPPÄNEN, "Serpent – a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code," *VTT Technical Research Centre of Finland, Espoo, Finland* (2012).
6. E. FRIDMAN and J. LEPPÄNEN, "On the use of the Serpent Monte Carlo code for few-group cross section generation," *Annals of Nuclear Energy*, **38**, *6*, 1399–1405 (Jun. 2011).
7. V. VALTAVIRTA, J. LEPPÄNEN, and T. VIITANEN, "Coupled neutronics-fuel behavior calculations in steady state using the Serpent 2 Monte Carlo code," *Annals of Nuclear Energy*, **100**, 50–64 (Feb. 2017).
8. J. LEPPÄNEN, M. PUSA, T. VIITANEN, V. VALTAVIRTA, and T. KALTIAISENAHO, "The Serpent Monte Carlo code: Status, development and applications in 2013," *Annals of Nuclear Energy*, **82**, 142–150 (Aug. 2015).
9. M. B. CHADWICK ET AL., "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," *Nuclear Data Sheets*, **107**, *12*, 2931–3060 (Dec. 2006).
10. A. LINDSAY, K. HUFF, and A. RYKHLEVSKII, "Arfc/Moltres: Initial Moltres Release," *Zenodo* (Jun. 2017).