

Molten Salt Tritium Breeding Materials in Fusion Reactors: A Neutronic Comparative Analysis for ITER

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Abstract

This study investigates the effects of varying tritium breeding materials and their lithium enrichment rates on the Tritium Breeding Ratio (TBR) and Energy Multiplication Factor (M) within the tritium breeding zone of a fusion reactor. The magnetic fusion reactor model was developed based on the geometric and plasma parameters of the International Thermonuclear Experimental Reactor (ITER), ensuring a realistic representation of current fusion reactor designs. ITER-grade stainless steel (SS 316 LN-IG) was selected as the first wall material due to its excellent mechanical properties, high resistance to radiation damage, and compatibility with hightemperature environments. The coolant and tritium breeding materials considered in the blanket included natural lithium, lithium fluoride (LiF), lithium nitride (Li₃N), FLiBe (LiF-BeF₂), and FLiNaBe (LiF-NaF-BeF₂). These materials were chosen for their ability to facilitate tritium breeding while maintaining thermal and neutronic efficiency. Neutron transport calculations and geometric modeling were performed using the widely recognized 3D simulation tools MCNP5 and TopMC, which employ the continuous-energy Monte Carlo method. The simulations utilized built-in continuous-energy nuclear and atomic data libraries, along with the Evaluated Nuclear Data File (ENDF) system (ENDF/B-V and ENDF/B-VI), ensuring reliable and validated results. The results highlight the importance of material selection and enrichment optimization in achieving efficient tritium breeding and energy production. FLiBe, in particular, shows promise for future fusion reactor designs due to its superior performance in terms of TBR and M. These findings provide valuable insights for the development of sustainable and high-performance fusion reactors, contributing to the global pursuit of clean and virtually limitless energy.

Full Text

Preamble

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Key Words: ITER, Magnetic Fusion Reactor, Tritium Breeding Ratio, Energy Multiplication Factor, Neutronic Analysis

1. Introduction

In the contemporary era, sustainable technological advancements and meeting humanity's ever-increasing demands are intrinsically linked to energy production and utilization. The exponential growth of human populations globally, together with processes of industrialization and urbanization, has resulted in an unprecedented rise in energy demands, making energy a pillar of economic and social development. Researchers and scientists are intensively exploring

both conventional and alternative energy supplies to cope with this challenge. Among these options, nuclear power represents one of the most important solutions—a sustainable, low-carbon, and highly efficient method of energy production. The last century has seen significant scientific efforts in developing nuclear energy technologies, which play a crucial role in meeting global energy requirements while minimizing environmental impacts, thereby setting the stage for advancements in fusion energy.

Compared to renewable energy production methods, nuclear energy provides a consistent and substantial amount of energy throughout the day, offering consumers a stable supply. Relative to fossil fuel-powered plants, nuclear energy uses significantly less fuel, consumes fewer materials, and produces zero carbon emissions, making it a sustainable energy source. Today's nuclear power plants utilize fission reactions, in which energy is generated by splitting atomic nuclei. However, a significant factor limiting the sustainability of fission reactors is the limited availability of fuel reserves, such as uranium and plutonium. In addition, both short-lived and long-lived radioactive waste are generated during reactor operation; if not managed and stored according to established protocols, these wastes can lead to serious environmental consequences. Beyond the necessity of waste storage and associated environmental risks, high fuel supply costs significantly reduce the advantages of fission reactors.

Unlike fission reactors, fusion reactors have significant potential to meet the need for sustainable nuclear energy because the fuel used in these reactors is almost unlimited. The abundance and easy accessibility of fusion fuel, as well as the absence of risks such as reactor meltdown or loss of control, have encouraged scientists and engineers to conduct extensive research on the feasibility of fusion technology. Studies conducted in the 1920s investigated the fundamental principles of fusion reactions and demonstrated that the energy generated in stars originates from these reactions [1]. This theory was later strengthened by mathematical models developed by Robert D'Escourt Atkinson and Fritz Houtermans, which revealed that the energy source in stars is nuclear fusion [2]. These studies further demonstrated that fusion reactions, while dependent on extremely high temperatures in stars, could also be carried out on Earth. Such early investigations provided significant momentum for the feasibility and development of fusion reactors.

In 1950, Andrei Sakharov and Igor Yevgenyevich Tamm proposed the concept of TOKAMAK (Toroidal Camera and Magnetic Coil), a type of magnetic confinement fusion device [3]. Shortly afterward, in 1951, Lyman Spitzer developed the Stellarator device, while Richard F. Post and Gersh Budker independently presented the concept of the magnetic mirror [4]. The TOKAMAK concept emerged as a significant breakthrough in magnetic confinement systems in the late 1960s thanks to experimental studies conducted by Lev Artsimovich. Following this development, TOKAMAK gained priority in research and development as the most suitable approach for achieving controlled nuclear fusion. Today, magnetic confinement fusion continues to be the dominant methodology

in fusion reactor designs, with intensive research being conducted on three basic configurations: TOKAMAK, Stellarator, and Magnetic Mirror systems.

In the early 1980s, comparative experiments between TOKAMAK and Magnetic Mirror configurations were conducted at the Princeton Plasma Physics Laboratory to evaluate the technological feasibility of these systems. These studies demonstrated that the TOKAMAK configuration was far more compatible with the operational requirements of fusion reactor technologies, establishing it as the preferred design [5]. The International Thermonuclear Experimental Reactor (ITER), which builds on decades of advances in magnetic confinement physics and plasma stability, represents the most advanced implementation of the tokamak concept [6]. ITER, the world's largest fusion experiment, aims to demonstrate the feasibility of deuterium-tritium (D-T) fusion as a sustainable energy source, targeting a tenfold energy gain ($Q \geq 10$) through improved plasma confinement [7]. The ITER design incorporates advances in materials engineering and superconducting magnet technology, with a primary focus on achieving sustained fusion combustion—a vital step toward practical fusion energy [8]. The ITER Project has continued to progress despite geometrical incompatibilities and corrosion issues in some components. A new project plan has been determined, system installations have been completed while repairs are ongoing, and most major components have been delivered. Initial experimental work is planned to begin in 2034, with the deuterium-tritium phase postponed to 2039 [9]. Developed through international collaboration, ITER builds on knowledge gained from previous tokamak experiments such as the Joint European Torus (JET), which broke records in plasma performance [10], and the Experimental Advanced Superconducting Tokamak (EAST), which has contributed to steady-state high-confinement plasma research [11].

One of the main challenges for deuterium-tritium (D-T) fueled reactors is the ability to produce tritium in a self-sufficient manner. Since tritium is both rare and radioactive, it must be produced continuously in the breeding blanket to sustain the fusion process. This production relies on neutron-lithium interactions within the blanket and requires carefully designed systems that optimize neutron utilization, thermal management, and material performance [12]. The success of this process directly impacts the reactor's long-term operational capability and its potential as a commercially sustainable energy source. To overcome tritium production challenges, extensive research is being conducted to optimize tritium breeding materials (TBM) and maximize the tritium breeding ratio (TBR) in fusion reactor blankets. Liquid tritium breeders such as lithium-lead (LiPb) have traditionally been preferred due to their high tritium production potential. However, concerns about polonium production via neutron activation have increased interest in lead-free alternatives such as molten salts and solid breeders [13-14-15].

Among these options, lithium fluoride-beryllium fluoride (FLiBe) and lithium fluoride (LiF) stand out due to their compatibility with high neutron flux environments, low long-term activation levels, and absence of polonium-related

safety risks [16-17]. Natural lithium (Li) and lithium nitride (Li_3N) have also been investigated due to their high lithium content and relatively simple tritium extraction methods. However, challenges such as neutron moderation efficiency, thermal-hydraulic properties, and chemical stability under irradiation remain active research areas [18-19-20]. Recent neutronic simulations have shown that FLiBe-based blankets can achieve tritium breeding ratios (TBR) above 1.1 in single-fluid configurations, particularly when combined with beryllium neutron multipliers, meeting the minimum requirement for fuel self-sufficiency [21]. Studies have demonstrated that to ensure tritium self-sufficiency in fusion reactors, the TBR value must exceed at least 1.05 [22]. Meeting this requirement necessitates optimizing the thickness and density of the first wall material, lithium enrichment levels, and blanket design to enhance neutron capture and tritium production efficiency. Lithium enrichment represents another effective method to increase tritium production, as it increases the density of the ^6Li isotope in breeding materials, thereby boosting TBR and enabling a more efficient and sustainable fuel cycle. Tritium production studies conducted for the DEMO fusion reactor determined that increasing ^6Li isotope density in the breeding zone is a key strategy [24].

After ensuring sustainable tritium production, design optimizations must be made to ensure that the energy produced exceeds the energy consumed. In this context, the reactor blanket structure must effectively capture neutron energy and convert it into useful forms. This conversion capability is expressed by the energy multiplication factor (M), which has been examined across different reactor concepts in the literature. In a study using the Helium-Cooled Lithium Lead Blanket concept in the DEMO fusion reactor, this value was calculated to be 1.17 [25]. In another study using the Helium-Cooled Pebble Bed Blanket concept, the energy multiplication factor was calculated to be 1.22 [26].

In addition to ensuring tritium self-sufficiency and maximizing the energy multiplication factor, selecting durable materials for the first wall structure is critical for fusion reactor success. Among available options, austenitic stainless steel SS 316 LN-IG (ITER grade) stands out due to its superior mechanical strength, radiation resistance, and ability to withstand extreme fusion environment conditions. This material, widely used in ITER, is preferred for the first wall due to its stability at high temperatures and its reduction of adverse effects such as swelling and embrittlement under radiation.

The first wall, directly exposed to plasma, must withstand harsh conditions including extreme thermal loads, neutron radiation, and particle bombardment; therefore, material selection is crucial for reactor durability and safety. SS 316 LN-IG is a low-carbon, nitrogen-strengthened 316 stainless steel specifically designed to endure these conditions. Its ability to mitigate radiation-induced swelling and embrittlement, combined with excellent weldability and high fracture toughness, makes it highly suitable for large-scale fusion applications such as ITER's blanket modules and divertor components [27].

2.1. Description of Magnetic Fusion Reactor Geometry

Figure 1 [Figure 1: see original paper] shows the three-dimensional cross-sectional geometry and main components of the magnetic fusion reactor. The geometry was created using the TopMC program, referencing ITER design parameters. The model includes essential reactor components such as the vacuum vessel, blanket, divertor, toroidal and poloidal field coils, central solenoid, thermal shield, and tritium breeding modules.

The materials and functional roles of these main reactor components are summarized in Table 1, which provides an overview of selected materials and their application areas in the modeled fusion reactor based on ITER design principles. Figures 2 and 3 [Figure 2: see original paper][Figure 3: see original paper] illustrate the poloidal and toroidal cross-sectional views of the magnetic fusion reactor modeled in MCNP5.

In these models, the plasma region is defined using ITER's deuterium-tritium (D-T) plasma parameters, featuring a low aspect ratio with a major radius of 6.2 m and a minor radius of 2 m. The plasma chamber is enclosed by a layered structure comprising, from innermost to outermost: the first wall, divertor, tritium breeding zone, neutron multiplier zone, reflector zone, thermal shield, vacuum vessel, and magnetic coils. Figure 4 [Figure 4: see original paper] shows the thickness of the blanket structure layers in the modeled reactor.

2.1.1. Plasma Chamber

The plasma chamber serves as the confinement region for plasma generated by deuterium-tritium (D-T) fusion reactions. High-energy neutrons produced in the plasma region during these reactions interact with the first wall. In the model, the neutron source is represented based on ITER's plasma parameters.

2.1.2. First Wall

The first wall is the interior surface of the tokamak, lying closest to the plasma and acting as the initial barrier that faces intense heat and particle flux generated during fusion reactions. Selecting appropriate materials for the first wall is therefore critical to ensure structural integrity and performance under extreme conditions. The first wall material must resist high temperatures and intense neutron flux while possessing excellent hardness, corrosion resistance, and a low neutron absorption cross-section to minimize adverse effects on the reactor's neutron economy. This study adopted a solid first wall design utilizing SS 316 LN-IG as the structural material due to its superior mechanical and neutronic properties.

2.1.3. Divertor

The divertor is a vital component in fusion reactors, particularly in TOKAMAK-type systems. Its primary functions include maintaining plasma purity by pre-

venting contact with the blanket structure and evacuating fuel particles from the plasma. These roles are essential for ensuring efficient and safe reactor operation.

2.1.4. Tritium Breeding Zone

Fusion reactors employ a dual-coolant system designed to facilitate both efficient heat transfer and tritium production. The primary coolant absorbs heat generated within the reactor and transfers it to a secondary coolant loop for energy conversion while simultaneously serving as the medium for tritium breeding, where lithium isotopes (^6Li and ^7Li) undergo neutron-induced reactions (n, α) and ($n, n\alpha$) to generate tritium (^3H). The selection of the primary coolant is a key design consideration that must meet several essential criteria: high lithium density to maximize tritium production; high specific heat and thermal conductivity for effective heat removal; low density and viscosity to improve flow dynamics; minimal corrosion and erosion effects; a high boiling point and low melting point for stable operation; a low neutron absorption cross-section to optimize neutron economy; and cost-effectiveness to support large-scale deployment.

In this study, molten salts—including natural lithium (Li), lithium fluoride (LiF), lithium nitride (Li_3N), FLiBe ($\text{LiF}-\text{BeF}_2$), and FLiNaBe ($\text{LiF}-\text{NaF}-\text{BeF}_2$)—were evaluated as primary coolant candidates due to their advantageous thermal and neutronic characteristics [28]. Their high lithium content, excellent thermal stability, and low neutron absorption make them well-suited for tritium breeding, while their compatibility with structural materials and ability to sustain high operating temperatures strengthen their potential for use in magnetic fusion reactor systems.

2.1.5. Neutron Multiplier Zone

The neutron multiplier zone is a critical component for enhancing tritium production, improving neutron economy, and ensuring a sustainable fuel cycle in fusion reactors. This zone amplifies the number of neutrons generated during D-T fusion reactions, thereby optimizing tritium breeding. In this study, Be12Ti was selected as the neutron multiplier material due to its favorable neutronic properties [29].

2.1.6. Reflector

The reflector layer redirects neutrons escaping from the coolant zone back into the reactor, increasing the likelihood of neutron interactions within the molten salt-fuel mixture. This layer minimizes neutron leakage and supports tritium breeding. In this study, graphite, which exhibits minimal neutron interaction, was used as the reflector material.

2.1.7. Thermal Shield

The thermal shield is designed to protect the ultra-cold superconducting magnets from excessive nuclear heating, radiation damage, and neutron flux while ensuring that radiation exposure to diagnostic tools and maintenance equipment remains within acceptable limits. The shield mitigates temperature variations, as superconducting magnets in TOKAMAK reactors operate at cryogenic temperatures (4 K). Each watt of thermal energy deposited in the magnets by neutrons and gamma rays requires approximately 500 watts of cooling energy to maintain operational stability [30].

2.1.8. Vacuum Vessel

The vacuum vessel serves as a confinement barrier in magnetic fusion reactor designs, ensuring minimal heat accumulation in specific regions, particularly magnetic field coils. By eliminating isotopes in these areas, heat transfer via convection and conduction is prevented. In the modeled reactor, a vacuum layer was incorporated between the insulation layer and the magnets to protect them from heat-induced degradation.

2.1.9. Magnetic Coils

Superconducting magnets are employed in magnetic fusion reactors to confine plasma within the reactor. Positioned in the outermost layer, these magnets generate magnetic fields that prevent plasma dispersion. Each magnet type serves a distinct purpose: a central solenoid functions as a large transformer to induce and sustain strong plasma currents during extended pulses; six horizontal poloidal field coils positioned outside the toroidal magnet structure control plasma shape and stability; and eighteen D-shaped vertical toroidal field coils surround the vacuum vessel, creating a magnetic bottle for plasma confinement. In this study, Nb3Sn and NbTi were selected as magnet materials based on the specific magnetic field requirements of each coil system.

3. Simulation Tools

In this study, the simulation tools MCNP and TopMC were used sequentially. The geometry designed in MCNP was tested in the TopMC program, and after making necessary adjustments, it was recreated as an MCNP input file. This generated input file served as a common input for both MCNP and TopMC, and simulation results were verified by ensuring consistency between output files produced by both programs.

3.1. MCNP

MCNP (Monte Carlo N-Particle) is a program used to model the transport of neutrons, photons, electrons, and other particles using Monte Carlo techniques. It is widely applied in nuclear engineering, radiation protection, and

various fields requiring particle transport analysis. The code is developed and maintained by Los Alamos National Laboratory (LANL) in the United States. The fifth version, MCNP5, leverages the Monte Carlo method, a statistical technique that simulates particle behavior by tracking individual trajectories through defined geometry [31]. This method is particularly beneficial for simulating complex systems and is advantageous for neutron transport problems where deterministic approaches may struggle with intricate geometries and material interactions.

MCNP5 employs a continuous-energy Monte Carlo method, meaning it doesn't rely on predefined energy groups but instead tracks particles across a seamless energy range. This is especially important for accurately modeling neutron behavior, as neutrons span a wide energy spectrum in many nuclear applications. Additionally, MCNP5's three-dimensional modeling capabilities enable detailed simulation of complex geometries, providing users with flexibility to accurately represent intricate systems. This makes MCNP5 a valuable resource for researchers and engineers working in reactor physics, radiation shielding, medical physics, and environmental radiation transport studies. Overall, MCNP5 serves as a robust tool for predicting and analyzing particle interactions in various environments.

3.2. TopMC

TopMC (Multifunctional Program for Neutronic Computing, Nuclear Design and Safety Assessment) is an advanced nuclear design software developed by the FDS (Fusion Design and Simulation) Consortium over more than thirty years. TopMC, an improved and extended version of SuperMC, serves as a large-scale tool for performing comprehensive neutronic calculations. Its main function is radiation transport calculations covering all neutronic processes such as depletion, radiation source term analysis, dose assessment, biohazard analysis, material activation, and transmutation. TopMC stands out with its high efficiency, precision, and multi-physics capabilities, offering accurate analytical modeling and visualization tools [32]. It also provides virtual simulation features, intelligent nuclear design, and powerful safety assessment functions. Although primarily used in the design and safety analysis of nuclear energy systems, TopMC also finds application in various nuclear technology fields such as radiation medicine and nuclear detection.

4.1. Tritium Breeding Ratio

The tritium breeding ratio is defined as the ratio of tritium produced in the blanket structure of a fusion reactor to tritium consumed in the plasma. Tritium, a key isotope for deuterium-tritium (D-T) fusion reactions, is not naturally abundant and must be continuously bred within the reactor's blanket to sustain the fusion process. Due to its radioactive instability and short half-life (approximately 12.3 years), tritium must be utilized shortly after production. If stored as a reserve, the required TBR for reactor operation increases over time

to account for decay and other losses. To ensure sufficient tritium production and sustainable fusion reactions, studies indicate that the TBR must be at least 1.05.

Tritium production in magnetic fusion reactors relies on complex interactions between thermal and fast neutrons with lithium isotopes. Lithium exists in two primary isotopes: ${}^6\text{Li}$ (7.6% natural abundance) and ${}^7\text{Li}$ (92.4% natural abundance). Tritium generation is governed by two key nuclear reactions: the exothermic ${}^6\text{Li} (n, t)$ reaction, where thermal neutrons interact with ${}^6\text{Li}$ to produce tritium, and the endothermic ${}^7\text{Li} (n, t)$ reaction, where fast neutrons interact with ${}^7\text{Li}$ to yield tritium. These reactions are fundamental to maintaining a sustainable tritium supply essential for fueling fusion reactions. The ${}^6\text{Li}$ isotope exhibits a significantly higher propensity for (n, t) reactions with thermal neutrons compared to ${}^7\text{Li}$, making it pivotal in determining the TBR. The enrichment ratio of ${}^6\text{Li}$ and the thickness of the coolant layer are critical factors influencing TBR, as they directly affect neutron capture efficiency and tritium production rate. The TBR results obtained as a function of ${}^6\text{Li}$ enrichment are shown in Figure 5 [Figure 5: see original paper].

4.2. Energy Multiplication Factor

The energy multiplication factor (M) is a key parameter used to evaluate the energy performance of the fusion reactor blanket system. It is defined as the ratio of total energy stored or recovered in the system to the kinetic energy of incident fusion neutrons. During fusion reactions, not all released energy is retained in the system—energy is lost through escaping neutrons, alpha particles, and gamma radiation. Since neutrons are uncharged, they travel beyond the plasma and deposit their energy in surrounding materials. To achieve net thermal power generation, the energy recovered from these reactions must exceed the energy initially carried by the plasma, making a sufficiently high energy multiplication factor essential. For D-T fusion systems, a minimum M value of 1.2 is generally considered necessary to offset system losses and contribute meaningfully to thermal energy output [33].

A well-designed blanket system must optimize these reactions to balance both tritium production and thermal energy recovery. Additionally, materials like beryllium, used as neutron multipliers, can improve neutron economy and enhance both the energy multiplication factor and tritium breeding ratio. Geometry, material selection, and neutron transport characteristics all influence how effectively the reactor can utilize fusion neutron energy. In calculating the energy multiplication factor, the two most significant factors in terms of energy production and consumption are the exothermic ${}^6\text{Li} (n, \alpha) T$ and endothermic ${}^7\text{Li} (n, \alpha n) T$ reaction energies. Therefore, the energy multiplication factor is calculated as follows:

$$M = 1 + 4.784 \times T_6 - 2.467 \times T_7$$

In this equation, the values T_6 and T_7 represent the tritium production rates of the ^6Li and ^7Li isotopes, respectively. The energy multiplication factor results from this study are shown in Figure 6 [Figure 6: see original paper].

5. Conclusion

In this study, detailed neutronic simulations were performed to assess the influence of different tritium breeding materials and various levels of lithium enrichment on the overall performance of the fusion reactor blanket system. Considering geometrical and operational constraints, calculations were carried out with a three-dimensional code for a system modeled on the ITER reference design. The input file created in the TopMC program was executed in both MCNP5 and TopMC, and the consistency of results confirmed the reliability of the neutronic calculations.

The blanket layout was studied under steady-state plasma conditions, with special attention to key performance parameters including TBR and M. Tritium production increased in simulations as lithium enrichment was raised to an optimum level, followed by a decrease. This non-linear behavior can be attributed to lithium's isotopic structure. While increasing enrichment raises the quantity of ^6Li , which generates tritium directly through the exothermic $^6\text{Li}(n,\alpha)\text{T}$ reaction, it also reduces the loading of ^7Li , which serves as a secondary neutron moderator and contributes to neutron economy through the $^7\text{Li}(n,n\alpha)\text{T}$ reaction. Low ^7Li levels decrease neutron moderation, affecting the thermal neutrons needed to sustain tritium breeding reactions. In contrast, the energy multiplication factor shows a consistent upward trend with increasing ^6Li content, as the reaction cross-section of $^6\text{Li}(n,\alpha)\text{T}$ is significantly higher at lower neutron energies.

Analysis of the results revealed that FLiNaBe and LiF exhibited sub-threshold neutronic performance with respect to the required TBR limit. Although FLiBe succeeded in exceeding the tritium breeding ratio within a moderate enrichment range (20-60%), it fell short of requirements at lower and higher enrichment levels, indicating sensitivity to lithium enrichment. Natural lithium and lithium nitride (Li_3N) also failed to meet the required threshold, even at 90% and 50% enrichment, respectively. These results are largely attributable to their unfavorable moderation characteristics and lower neutron economy compared to enriched FLiBe mixtures. In terms of energy multiplication, FLiBe consistently delivered the highest energy multiplication factor values across the enrichment spectrum, particularly in configurations where the tritium breeding ratio remained above the minimum threshold. This demonstrates FLiBe's dual effectiveness in enhancing both tritium production and thermal energy generation.

Consequently, based on simulation results using ITER-based geometry and plasma parameters, FLiBe appears to be the most suitable tritium breeding material for future magnetic fusion reactor concepts. Its ability to support self-sustaining fuel cycles while delivering higher thermal output makes it a strong

candidate for integration into environmentally sustainable and economically viable magnetic fusion systems. These findings, particularly regarding FLiBe' s performance, are expected to inform material selection strategies and blanket design optimizations in upcoming fusion energy projects.

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Note: Figure translations are in progress. See original paper for figures.

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