Neutron Transport and Tritium Breeding Modelling in Nuclear Fusion Reactor Breeder Blankets

MPhys Project Report

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November 8, 2025

Abstract

The pursuit of practical nuclear fusion is focused on the deuterium-tritium (D-T) fuel cycle, widely considered the most feasible pathway for near-term power generation. A critical challenge, however, is the reliance on tritium, a radioactive isotope with an extremely limited external supply, necessitating a self-sufficient fuel cycle. The D-T fusion reaction produces most of its energy as 14.1 MeV neutrons, which can in turn be used to regenerate tritium through neutron-lithium interactions. The reactor subsystem that performs this function—the breeder blanket—is therefore essential for the viability of the D-T fuel cycle. It must simultaneously extract heat, shield reactor components, and maintain tritium self-sufficiency. This project applies Monte Carlo neutron transport simulations using `OpenMC` to investigate the neutronic performance of advanced breeder blanket designs, including heterogeneous and functionally graded geometries. The study aims to quantify how variations in material composition and spatial structure influence the tritium breeding ratio (TBR) and neutron flux profiles, and explores the potential for automated optimisation of blanket parameters through computational frameworks. The outcomes will inform the feasibility and efficiency of next-generation blanket concepts relevant to future magnetic confinement fusion reactors such a DEMO and STEP.

1. INTRODUCTION

The pursuit of practical nuclear fusion represents one of the most ambitious and potentially transformative scientific endeavours of the twenty-first century. As global energy demand continues to rise and the environmental impacts of fossil fuel use become ever clearer, fusion offers the prospect of a near-limitless, low-carbon energy source. Fusion energy aims to replicate, on Earth, the processes that power the Sun — combining light nuclei to release energy through mass-energy conversion. Unlike conventional nuclear fission, fusion promises inherent safety, reduced long-lived radioactive waste, and abundant fuel sources.

Among the various fusion reactions studied, the deuterium-tritium (D-T) reaction has emerged as the most viable for near-term applications due to its relatively high cross-section at achievable plasma temperatures and its favourable energy yield. However, the practical realisation of a D-T reactor introduces challenges that extend far beyond plasma confinement and heating. Chief among these is the supply of tritium, a radioactive isotope that does not occur naturally in significant quantities and must be produced artificially.

This challenge has led to the development of the breeder blanket concept — an integrated structure surrounding the plasma that captures energetic neutrons produced in fusion reactions and uses them to generate tritium through interactions with lithium. In addition to tritium production, breeder blankets also serve several critical roles: moderating neutron flux, capturing energy for conversion to electricity, and protecting reactor components from radiation damage.

Understanding the behaviour of neutrons within the blanket region is therefore central to the success of any D-T fusion system. Computational modelling of neutron transport, energy deposition, and tritium breeding provides vital insights into how different blanket materials and geometries perform under fusion-like conditions. These neutronics studies inform the design and optimisation of test blanket modules and full-scale reactor concepts.

This project contributes to that effort by using advanced Monte Carlo simulations to model neutron interactions within candidate breeder blanket materials. Through this, it aims to identify promising compositions and geometries capable of sustaining tritium self-sufficiency in future fusion power plants.

2. THEORY

2.1. Fundamentals of Nuclear Fusion

Nuclear fusion is the process by which two light atomic nuclei combine, or "fuse," to form a single, heavier nucleus [1]. This reaction is the primary process powering stars, and it is a candidate for future terrestrial energy generation.

The release of energy in fusion is a direct consequence of **nuclear binding energy**. The nucleons (protons and neutrons) in a nucleus are held together by the strong nuclear force. The binding energy is the energy required to disassemble the nucleus into its separate components. Conversely, when a nucleus is formed, this amount of energy is released.

Crucially, the binding energy *per nucleon* is not constant across all elements. Lighter nuclei,

such as hydrogen isotopes, are relatively loosely bound. Nuclei in the "medium-mass" range, like helium-4 or iron, are much more tightly bound.

Therefore, when two light nuclei fuse to form a heavier, more tightly bound nucleus, the total binding energy of the system *increases*. This surplus energy is released during the reaction. This gain in binding energy corresponds to a reduction in the total rest mass of the system. This difference, known as the **mass defect** (Δm), is not truly "lost" but is converted into energy (E) according to Einstein's principle of mass-energy equivalence [1].

This relationship is famously expressed by the equation $E = mc^2$, or more specifically for a reaction, as a release of energy Q (the "Q-value"):

$$Q = \left(\sum m_{\text{reactants}} - \sum m_{\text{products}}\right) c^2 = (\Delta m)c^2 \tag{1}$$

Because the speed of light squared (c^2) is an enormous constant, even a minuscule decrease in mass releases a tremendous amount of energy, typically in the form of kinetic energy of the products (e.g., neutrons, alpha particles) and/or high-energy photons (gamma rays).

For terrestrial power generation, the most promising reaction is that between the two heavy isotopes of hydrogen, deuterium (d) and tritium (t) [2, 3]:

$$\mathrm{d} + \mathrm{t} \longrightarrow \mathrm{n} + \alpha + 17.6MeV$$

This D-T reaction is the primary focus of mainstream fusion research, as it has a fusion cross-section significantly higher than other candidate reactions (such as D-D or D$-^3$He) (Fig. 1) [3]. This is mainly due to the stability of the final products linking to a higher Q value output [1].

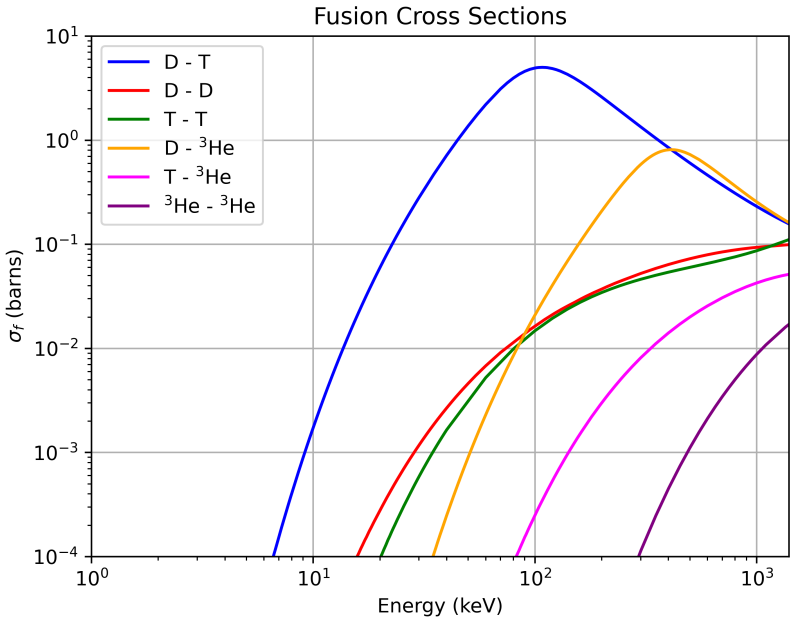

Figure 1: A comparison of fusion reaction reactivities total cross section σ as a function of ion temperature (keV) for the D-T, D-D, and D-^{3}He fuel cycles. The D-T reaction's cross section peaks at a lower temperature and is significantly larger than the alternatives, making it the most accessible reaction for current and near-term fusion devices.

Another important reason for D-T is the is the comparatively lower required input energy / temperature. To initiate fusion, the positively charged nuclei must be given enough kinetic energy to overcome their mutual electrostatic repulsion, known as the Coulomb barrier. This barrier will increase if the reactants have a more positive charge and so more electrostatic repulsion. This can exclude cycles like D-^{3}He as the required temperatures/energies are already high enough (hotter than the core of the sun). In Magnetic Confinement Fusion (MCF) devices, such as the **tokamak** [4], this is achieved by heating the D-T gas into a plasma state at temperatures exceeding 100 million Kelvin. The hot plasma is then confined by powerful magnetic fields, preventing it from touching the reactor walls. The 17.6 MeV of energy released is partitioned between the two products: the alpha particle (α, a helium nucleus) carries 3.5 MeV, while the neutron (n) carries 14.1 MeV [3].

This energy split is fundamental to the reactor's operation. The charged alpha particle remains trapped by the magnetic fields, depositing its energy into the plasma and helping to sustain its high temperature (a process known as "plasma burning"). The neutron, being electrically neutral, is un-bothered by the magnetic fields and escapes the plasma immediately, carrying 80% of the fusion energy with it [3].

2.2. Neutron Transport and Interactions

The 14.1 MeV neutron is the primary vehicle for both energy extraction and fuel production. Once it leaves the plasma, it travels into the surrounding structures, chiefly the **breeder blanket**. The study of its journey and interactions with the blanket materials is the domain of **neutron transport** [5].

As the neutron moves through matter, it interacts with atomic nuclei via two main processes: scattering and absorption. The probability of any specific interaction occurring is defined by the material's **microscopic cross-section (σ)**, a value that is highly dependent on the energy of the incident neutron [5]. These cross-sections are meticulously measured and compiled in comprehensive libraries such as the Evaluated Nuclear Data File (ENDF) [6].

Key interactions within the blanket include:

2.2.1. Scattering Interactions

The neutron collides with a nucleus and "bounces" off, transferring a portion of its kinetic energy to the nucleus. In **elastic scattering** $(\mathrm{n}, \mathrm{n}')$, kinetic energy is conserved. In **inelastic scattering** $(\mathrm{n}, \mathrm{n}')$, the neutron excites the nucleus, which then de-excites by emitting a gamma ray, resulting in a larger energy loss for the neutron. Both processes are crucial for **moderation**—slowing the fast 14.1 MeV neutrons down. This thermal energy, deposited in the blanket material, is what is ultimately extracted by a coolant to generate electricity.

2.2.2. Absorption Interactions

The neutron is captured by a nucleus. This can be a **radiative capture (n, γ)** event, where the nucleus emits a gamma ray. This is often a parasitic reaction, as it removes a neutron from the system that could have been used for breeding. Alternatively, the absorption can

induce **charged particle emission**, such as (n, p) or (n, α) reactions. This is the fundamental mechanism used for tritium breeding [5].

2.3. Tritium Breeding and Neutron Multiplication

The primary nuclear function of the blanket is to use the fusion neutrons to "breed" new tritium fuel. This is accomplished by bombarding lithium isotopes with the neutrons. There are two reactions that produce tritium:

$$^{6}\mathrm{Li} + \mathrm{n} \longrightarrow \alpha^{+} + \mathrm{t} + 4.8MeV \tag{2}$$

$$^{7}\mathrm{Li} + \mathrm{n} \longrightarrow \alpha^{+} + \mathrm{t} + \mathrm{n}' - 2.5MeV \tag{3}$$

The ^{6}Li reaction is exothermic and has a very large cross-section for low-energy (thermal) neutrons, making it the primary breeding reaction of interest [7]. The ^{7}Li reaction is endothermic, requiring high-energy neutrons (a "threshold" reaction), and is generally less effective.

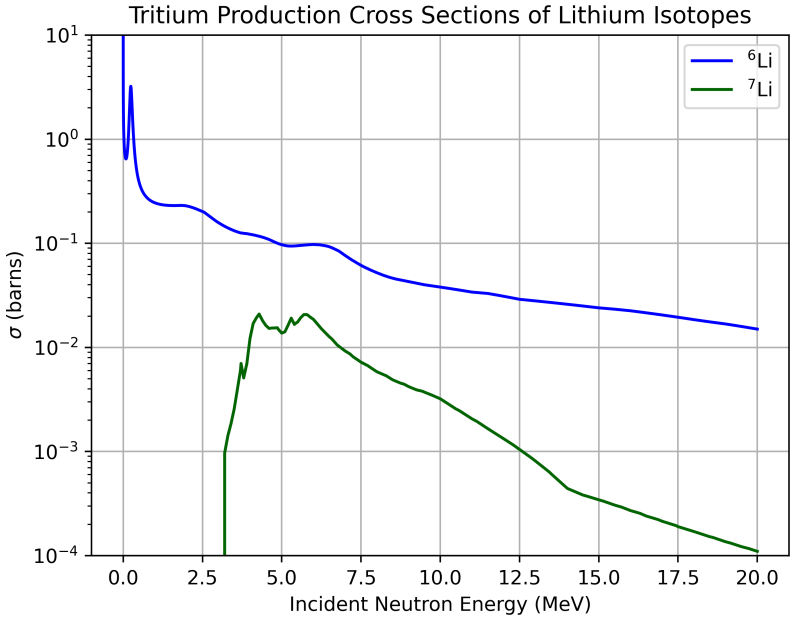

Figure 2: Neutron cross-sections for the primary tritium breeding reactions, $^{6}\mathrm{Li}(\mathrm{n}, \alpha)\mathrm{t}$ and $^{7}\mathrm{Li}(\mathrm{n}, \alpha\mathrm{t})\mathrm{n}'$, as a function of incident neutron energy. The ^{6}Li cross-section is dominant at low (thermal) energies, while the ^{7}Li reaction is a threshold reaction requiring high-energy neutrons.

The critical metric for the blanket's success is the **Tritium Breeding Ratio (TBR)**, defined as the ratio of tritium atoms produced in the blanket to the tritium atoms consumed in the plasma [8]. Due to inevitable fuel cycle losses (e.g., incomplete plasma burn-up, decay during extraction), the blanket must breed more tritium than is consumed. To achieve a self-sufficient fuel cycle, a TBR > 1.0 is mandatory, with most reactor designs targeting a value of 1.1 or higher [9, 10].

This presents a "neutron economy" challenge. The D-T reaction produces one neutron, and the primary ^{6}Li breeding reaction consumes one neutron [11]. This leaves no margin for neutrons

that are inevitably lost, either by leaking out of the blanket or through parasitic absorption in structural materials (like steel) [11].

To overcome this deficit, the blanket must include a **neutron multiplier** [12, 7]. These are materials that undergo an **(n, 2 n)** reaction, where one high-energy incident neutron strikes a nucleus and causes two neutrons to be emitted. The two most viable multiplier materials are Beryllium (Be) and Lead (Pb) [7].

$$^{9}\mathrm{Be} + \mathrm{n} \longrightarrow {}^{8}\mathrm{Be} + 2\,\mathrm{n} \longrightarrow 2\,\alpha^{+}\,2\,\mathrm{n}$$

$$^{208}\mathrm{Pb} + \mathrm{n} \longrightarrow {}^{207m}\mathrm{Pb} + 2\,\mathrm{n}$$

By incorporating these materials, the single 14.1 MeV fusion neutron can be multiplied into two or more lower-energy neutrons. These neutrons are then moderated (slowed down) within the blanket until they are at the optimal thermal energy to be captured by ^{6}Li, thus enabling a TBR significantly greater than one [7].

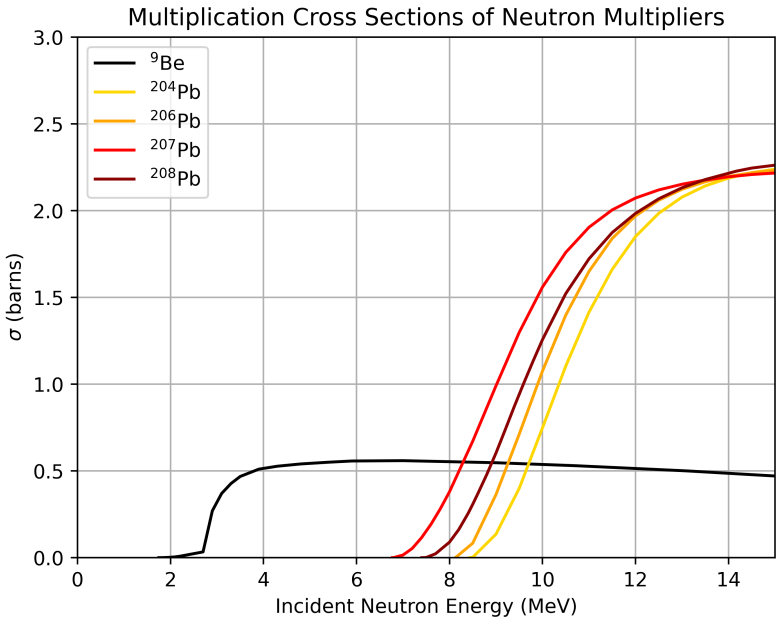

Figure 3: Neutron cross-sections for the (n, 2 n) neutron multiplication reactions in Beryllium (^{9}Be) and Lead (^{208}Pb). Both are threshold reactions that require high-energy neutrons, such as those from the D-T fusion reaction (14.1 MeV), to effectively multiply the neutron population.

3. LITERATURE REVIEW

3.1. The D-T Reaction and the Tritium Fuel Imperative

The deuterium-tritium (D-T) fusion reaction, $\mathrm{d} + \mathrm{t} \longrightarrow \mathrm{n} + \alpha^{+}\,17.6\,\mathrm{MeV}$, has been the leading candidate for first-generation fusion power plants since its potential was identified in the 1940s [2]. Its primary advantage lies in its high fusion cross-section (σ_f) at plasma temperatures

achievable with current technology, significantly higher than other candidates like D-D or D-^{3}He reactions. Furthermore, 80% of the energy (14.1 MeV) is carried by the emitted neutron, which allows for energy to be efficiently extracted from the plasma core [3].

This reliance on the D-T reaction, however, creates a fundamental logistical challenge: the fuel cycle is not self-contained. While deuterium is abundant in seawater, tritium is a radioactive isotope with a short half-life of 12.32 years and is not found in nature in any significant quantity. The world's current tritium supply is a by-product of heavy-water-moderated fission reactors, such as CANDU reactors. Multiple analyses of this supply chain have concluded that global stockpiles are extremely limited and face serious shortages [13, 14], *even without* the projected demand from a future fleet of fusion power plants.

Therefore, for fusion energy to be a sustainable and viable long-term power source, any commercial D-T reactor must breed its own tritium. This has led to the development of in-situ fuel production systems, known as **Tritium Breeder Blankets**.

3.2. Breeder Blanket: Concept, Function, and Evolution

A breeder blanket is a complex component surrounding the plasma-containing vacuum vessel. Its primary function is to intercept the 14.1 MeV fusion neutrons and use them to induce tritium-producing reactions in lithium. These are in reference to the two key breeding equations Eq. (2) and Eq. (3).

While ^{7}Li can breed, the ^{6}Li reaction is exothermic and possesses a much larger reaction cross-section for the thermalised neutrons dominant in a blanket, making it the primary breeding isotope.

The concept of a "breeder" blanket predates its application in fusion; it was first developed as a method to use fusion neutrons to produce fissile materials, such as ^{233}U and ^{239}Pu, for fission reactors [15, 16, 17]. Today, the design must also perform several other critical functions, including shielding the superconducting magnets from intense neutron radiation and extracting the fusion energy (via neutron thermalisation) for power conversion.

The key metric for a blanket's performance is the **Tritium Breeding Ratio (TBR)**, defined as the ratio of tritium atoms produced in the blanket to the tritium atoms consumed in the plasma. Due to inevitable losses from neutron capture in structural materials, decay, and incomplete fuel burn-up, a TBR significantly greater than 1.0 is required to achieve tritium self-sufficiency [9, 10].

However, the D-T reaction produces only one neutron, and the ^{6}Li reaction consumes one neutron. This leaves no margin for losses. To achieve a TBR > 1, most blanket designs must include a **neutron multiplier** material. The most effective materials for this are beryllium (^{9}Be) and lead (^{208}Pb), which undergo $(\mathrm{n}, 2\,\mathrm{n})$ reactions (spallation) when struck by high-energy fusion neutrons, effectively turning one incident neutron into two [7].

3.3. The Role of Neutron Multipliers

The D-T fusion reaction produces a single 14.1 MeV neutron, while the primary breeding reaction, $^6\mathrm{Li}(\mathrm{n}, \alpha)\mathrm{t}$, consumes one neutron. This 1-to-1 neutron economy leaves no margin for

inevitable losses due to parasitic absorption in structural materials or neutrons escaping the blanket. To achieve the required Tritium Breeding Ratio (TBR) greater than unity, a blanket must therefore incorporate a **neutron multiplier** [12].

Natural lithium itself has a minor neutron-multiplying reaction via the high-energy $(\mathrm{n}, \mathrm{n}'\mathrm{t})$ reaction with $^{7}\mathrm{Li}$, shown in Eq. (3). However this reaction is endothermic, consuming 2.5 MeV of energy, and its cross-section is insufficient on its own to guarantee tritium self-sufficiency [7]. This leads to a common consensus that dedicated neutron multipliers are required with the two primary candidates being Beryllium (Be) and Lead (Pb).

3.3.1. Beryllium Neutron Multipliers

Beryllium, specifically the isotope $^{9}\mathrm{Be}$, is an extremely effective neutron multiplier with a low energy threshold for its $(\mathrm{n}, 2\,\mathrm{n})$ reaction:

$$^{9}\mathrm{Be} + \mathrm{n} \longrightarrow {}^{8}\mathrm{Be} + 2\,\mathrm{n} \longrightarrow 2\,\alpha + 2\,\mathrm{n}$$

It is widely used in conceptual solid breeder designs, such as the Helium-Cooled Pebble Bed (HCPB) and Water-Cooled Pebble Bed (WCPB), often in the form of beryllium pebbles or beryllide ceramics ($\mathrm{Be_{12}Ti}$) [18, 19]. It is also a key component in the molten salt FLiBe ($2\,\mathrm{LiF} \cdot \mathrm{BeF_2}$) [20, 21]. However, beryllium has two major drawbacks: it is a scarce resource, and its dust is "ridiculously toxic" [22], posing significant safety, handling, and manufacturing challenges.

3.3.2. Lead Neutron Multipliers

Lead, typically natural lead or lead enriched in $^{208}\mathrm{Pb}$, is the other main multiplier candidate. It undergoes a high-energy $(\mathrm{n}, 2\,\mathrm{n})$ reaction:

$$^{208}\mathrm{Pb} + \mathrm{n} \longrightarrow {}^{207m}\mathrm{Pb} + 2\,\mathrm{n}$$

Lead's primary advantage is that it can be seamlessly integrated into a liquid breeder, forming the $\mathrm{Li_{17}Pb_{83}}$ eutectic alloy. This allows the material to serve as breeder, multiplier, and coolant simultaneously [23, 12]. While it avoids the toxicity issues of beryllium, lead is a high-Z (high atomic number) material. This means it can also be a source of parasitic neutron absorption, particularly for the low-energy thermal neutrons that are most effective for breeding with $^{6}\mathrm{Li}$. Furthermore, its activation by high-energy neutrons can lead to the production of long-lived radioisotopes, complicating waste disposal [24].

The choice of multiplier, therefore, represents a critical trade-off between neutronic efficiency, material toxicity, resource availability, and long-term waste management [7, 22].

3.4. Major Breeder Blanket Architectures

Blanket designs are broadly divided into two categories—liquid and solid—based on the phase of the lithium-bearing breeder material.

3.4.1. Liquid Breeder Concepts

Liquid breeders (LBs) are attractive because the breeding medium can simultaneously function as the coolant, simplifying the design and allowing for continuous tritium extraction outside the reactor [20].

3.4.1.1. Lithium-Lead (Li – Pb):

This is one of the most mature concepts, typically using the eutectic alloy $Li_{17}Pb_{83}$ [25, 23]. The lead acts as both a neutron multiplier and the primary component of the alloy, while the eutectic composition provides a low melting point, which is crucial for circulation [25]. This concept is the basis for the **Dual-Cooled Lithium-Lead (DCLL)** blanket, a primary candidate for the European DEMO reactor [26, 12]. A key challenge for all liquid metal blankets is magnetohydrodynamics (MHD), where the strong magnetic fields of the tokamak induce currents in the flowing metal, creating a drag force that inhibits circulation [12].

3.4.1.2. Molten Salts:

An alternative LB concept uses molten fluorine or chlorine salts. The most prominent example is **FLiBe ($\mathbf{2\,LiF \cdot BeF_2}$)**, which advantageously combines the breeder (LiF) and multiplier (BeF_2) into a single, low-conductivity fluid [20]. This is the reference design for the **Affordable Robust Compact (ARC)** reactor concept from MIT [21, 24, 27]. A wide variety of other salt compositions, including $LiF \cdot PbF_2$ and novel chlorine-based salts, are also under investigation to optimise breeding, temperature, and material compatibility [28, 29].

3.4.2. Solid Breeder Concepts

Solid breeders (SBs) use lithium-based ceramics, typically in the form of packed pebble beds, which eliminates MHD issues and offers high chemical stability [30, 31].

3.4.2.1. Materials and Design:

The leading candidate materials are lithium metatitanate (Li_2TiO_3) and lithium orthosilicate (Li_4SiO_4), often mixed with separate beryllium-based pebbles (e.g., $Be_{12}Ti$) as a multiplier [7, 32]. A review by [7] provides a comprehensive survey of these and other solid-phase options.

3.4.2.2. Implementations:

These materials form the basis of several major international designs. The **Chinese Fusion Engineering Test Reactor (CFETR)** is developing a **Water-Cooled Pebble Bed (WCPB)** blanket using $Li_2TiO_3/Be_{12}Ti$ pellets [19, 33]. European and Japanese DEMO concepts have focused on **Helium-Cooled Pebble Bed (HCPB)** designs, which are also being developed for ITER Test Blanket Modules [34, 18, 35].

The primary challenges for SB concepts are the complex engineering required for cooling (either with high-pressure helium or water) and the difficulty of extracting tritium, which must diffuse out of the solid ceramic and can be trapped in radiation-induced vacancies [36].

3.5. Neutronics Modelling and the Research Gap

Evaluating the TBR and other neutronic parameters of these complex designs is extremely difficult to do experimentally [37, 38]. While small-scale mockups provide crucial data on material properties and tritium release, they cannot replicate the full neutron spectrum and geometry of a power plant [37]. Consequently, the field relies heavily on computational modelling, particularly **Monte Carlo (MC) simulations**. The probabilistic nature of neutron transport—defined by scattering, absorption, and multiplication cross-sections—is ideally suited to the statistical sampling methods of MC codes [39, 5].

Modern neutronic toolchains are central to this research effort. The field increasingly utilizes state-of-the-art, open-source Monte Carlo codes, which have been validated against other established codes and shown to accurately reproduce TBR and neutron flux calculations for fusion systems [40, 41, 42, 43]. A significant hurdle in this process is the management of complex reactor geometries. Accurately translating detailed Computer-Aided Design (CAD) models into a format usable by the neutronics code is a well-known challenge, often requiring significant manual effort [44] and geometric simplification [28].

A review of the literature reveals that decades of research have narrowed the focus to a small selection of "safe" materials (e.g., Li-Pb, Li_4SiO_4, Li_2TiO_3) chosen not only for breeding but for their structural, chemical, and cost properties [11, 8]. This necessary pragmatism has left many other material combinations, particularly those in complex molten salt systems, comparatively unexplored [7].

However, this material-focused pragmatism is not the only factor limiting the current design space. A significant methodological gap exists. Past neutronic studies have typically been forced to choose between breadth and depth. On one hand, broad surveys like [7] provide an excellent "first principles" review of a wide range of breeder and multiplier materials. But to compare so many options, these studies must rely on simplified, often one-dimensional, models, which cannot capture the complex three-dimensional neutron transport effects within a realistic tokamak geometry.

On the other hand, studies focused on specific reactor concepts, such as the molten salt analysis for DEMO by [45] or the liquid breeder comparison for ARC by [28], provide vital, high-fidelity 3D analysis. However, their conclusions are inherently tied to the *fixed geometry* of that specific reactor design. These studies typically compare a handful of materials within a single "dedicated model," fixing crucial parameters like blanket thickness and structural fractions. Consequently, they can answer "What is the best material for *this* design?" but not "What is the best *combination* of material and geometry?" For example, such studies often present TBR as a function of ^{6}Li enrichment, but do not explore how varying the blanket thickness or material composition ratios would fundamentally change those results.

This limited scope was, until recently, a computational necessity. Manually creating and simulating thousands of unique, complex 3D CAD models for a full parametric sweep was computationally intractable. Recent advances in scriptable, parametric modelling workflows have fundamentally lowered this barrier, making it feasible to automatically generate and distribute simulations for vast libraries of reactor designs. Work by [46] has demonstrated the power

of this new toolchain by modelling *several* distinct geometries. While this provides an excellent proof-of-concept, but as an unpublished paper this foundational work represents an initial step and leaves a significant opportunity for a more comprehensive and systematic exploration, particularly regarding material composition.

This project aims to fill this gap. By leveraging an integrated modelling workflow, we will conduct a broad, systematic investigation of TBR performance. This work builds upon previous studies by moving beyond the 1D-vs-3D or material-vs-geometry trade-off. We will explore the *coupled design space* by systematically and simultaneously varying key parameters that are often fixed: ^{6}Li enrichment, blanket thickness, and material composition ratios in a realistic 3D geometry. This systematic parameter sweep will provide a comprehensive dataset to identify optimal *combinations* of parameters, identifying design points that previous, more narrowly-focused studies may have overlooked.

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4. METHODOLOGY

4.1. Modelling Neutron Transport: From Boltzmann to Monte Carlo

The physics of neutron interactions described in Section 3.5—including scattering, absorption, and multiplication—must be accurately modelled to determine the neutronic performance of a breeder blanket. The behaviour of the entire neutron population (or **neutron flux**) within the reactor geometry is formally governed by the **Boltzmann Transport Equation (BTE)**.

The BTE is fundamentally a particle balance equation. In conceptual terms, it states that the rate of change of neutrons in a specific volume of space, travelling in a specific direction with a specific energy, is equal to the sum of all neutron gains and losses. Gains come from neutrons scattering *into* that state from other states and from external sources (like the D-T plasma). Losses come from neutrons scattering *out* of that state, being absorbed (either parasitically or in a breeding reaction), or simply leaking out of the volume.

While comprehensive, the BTE is an complex integro-differential equation that is impossible to solve analytically for a three-dimensional, heterogeneous geometry like a fusion reactor. Therefore, a numerical approach is required. This project employs the **Monte Carlo (MC) method**, a stochastic technique that has become a cornerstone of neutron transport modelling since its development for neutronic simulations [39].

Instead of solving the BTE for the entire population at once, the MC method simulates the individual life histories of millions, or billions, of discrete particles [39]. In this work, each "particle" is a neutron. A simulation proceeds as follows:

1. A source neutron is "born" at the plasma, with an energy of 14.1 MeV and a random direction.

2. The code uses the material cross-section data [6] as a set of probability distributions to determine how far the neutron travels before its next interaction.

3. At the interaction site, the code again uses the probabilistic data to decide *what* happens: it may scatter (elastically or inelastically), be absorbed (e.g., by ^{6}Li), or cause a multiplication event (e.g., an (n, $_{2}$n) reaction in Beryllium or Lead).

4. The neutron's energy and direction are updated, and if it still exists (i.e., was not absorbed), the process repeats. If it was a multiplication event, a new, secondary neutron is added to the simulation to be tracked.

5. This "life history" continues until the neutron (and all its children) are "killed"—either by being absorbed or by escaping the model geometry.

By simulating a sufficiently large number of these individual histories, the averaged behaviour of all particles converges to a statistically robust solution of the BTE. This statistical approach allows for the estimation of key neutronic parameters, such as the spatial distribution of the neutron flux and, most critically for this project, the **Tritium Breeding Ratio (TBR)**.

4.2. Computational Workflow and Toolchain

As established in the Literature Review (Section 3), modern neutronics research relies on a toolchain of simulation and geometry codes. This project leverages this approach by using two key open-source tools: `OpenMC` and **Paramak**.

- `OpenMC`**:** All simulations in this project are performed using `OpenMC`, a state-of-the-art, open-source Monte Carlo transport code [40]. `OpenMC` is widely used in the fusion research community and has been extensively validated against other codes for complex fusion neutronics applications, demonstrating high accuracy in calculating parameters like TBR and volumetric heating [41].

- **Paramak:** To manage the complex reactor geometry, this project also uses **Paramak**. It is a Python-based CAD framework that automates the construction of parametric tokamak models compatible with `OpenMC` [44], and is a key contributer to this project in providing a fast paramaterised easy to access API to generate sweep of geometry features and a variety of fusion reactor designs.

4.3. Simulation Strategy and Parametric Study

To systematically explore the vast design space, this project implements a custom, automated simulation pipeline. This pipeline leverages the modular, scriptable nature of `Paramak` and `OpenMC`, enabling key geometry and material parameters to be varied programmatically. By structuring the simulation inputs as single functional arguments, the pipeline is explicitly designed for iterative loops, allowing for large-scale parametric sweeps.

The core workflow for each individual simulation follows a precise sequence:

1. **Geometry Generation:** `Paramak` generates a 3D reactor model (which uses a `CadQuery` backend [44]) based on a given set of input parameters (e.g., blanket thickness, component radii).

2. **Geometry Conversion:** This CAD model is converted into a DAGMC (Direct Accelerated Geometry Monte Carlo) unstructured mesh geometry, a format optimized for particle transport codes.

3. **Model Setup:** The DAGMC geometry is imported into `OpenMC`, where it is populated with the specified material definitions and assigned the D-T fusion neutron source distribution (14.1 MeV).

The overall research strategy is executed in two main phases. First, the pipeline's validity is established by modelling a basic, reference tokamak geometry. This initial step serves to benchmark the workflow, confirm physically sensible results, and establish initial neutronic trends.

Following this validation, a more comprehensive, multi-parameter study is performed. This second phase executes coupled simulations to explore how changes in one parameter (e.g., ^{6}Li enrichment) affect the optimal value of another (e.g., blanket thickness). The pipeline's architecture is designed for distributability, allowing these computationally intensive simulations to be run in parallel. This systematic sweep will be applied to three key reactor design archetypes, enabling an "agnostic" rating of certain features and the identification of robust design principles that hold true across different blanket concepts.

5. RESULTS

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Table 1: A summary of solid breeder materials, their properties, and calculated TBR. (Note: TBR values are placeholders to be populated.)

Material	**Li (molar %)**	ρ **(g/cm^3)**	**TBR**	**Reference**
Li_2O	66.66	2.10	x	[34]
Li_4SiO_4	44.44	2.40	x	[25]
Li_2TiO_3	33.33	3.43	x	[25]
Li_8PbO_6	53.33	4.28	x	[25]
Li_8SiO_6	53.33	2.20	x	[25]
Li_8CoO_6	53.33	2.47	x	[25]
Li_8GeO_6	53.33	2.64	x	[25]
Li_8ZrO_6	53.33	2.98	x	[25]
Li_8SnO_6	53.33	3.41	x	[25]
Li_8CeO_6	53.33	3.25	x	[25]
Li_6MnO_4	54.55	2.50	x	[25]
Li_6CoO_4	54.55	2.77	x	[25]
Li_6ZnO_4	54.55	2.86	x	[25]
$Li_6Zr_2O_7$	40.00	3.56	x	[25]
Li_5AlO_4	50.00	2.25	x	[25]
Li_5FeO_4	50.00	2.64	x	[25]
Li_4TiO_4	44.44	2.57	x	[25]
Li_4GeO_4	44.44	3.16	x	[25]
Li_2SiO_3	33.3	2.53	x	[34]
Li_2MnO_2	40.00	3.90	x	[25]

Table 2: A summary of liquid breeder materials, their properties, and calculated TBR. (Note: TBR values are placeholders to be populated.)

Material	**Ratio (molar %)**	**Li (molar %)**	ρ **(g/cm^3)**	**TBR**	**Reference**
Li	-	100	0.47	x	[28]
Li-Pb	17:83	17.00	11.00	x	[9]
$LiF-BeF_2$	2:1	28.57	2.04	x	[29]
$LiF-BeF_2$*	1:1	20.00	2.06	x	[29]
LiF	-	50.00	2.64	x	[25]
Li_3N	-	75.00	1.30	x	[25]
$LiF-PbF_2$	2:3	15.38	3.55	x	[29]
$LiF-BeF_2-NaF$	1:1:1	14.29	2.15	x	[29]
$LiF-NaF-KF$	46.5:11.5:42	20.17	2.02	x	[28]
$LiF-LiBr-NaBr$	20:73:7	46.50	3.16	x	[28]
$LiF-LiBr-NaF$	14:79:7	45.69	3.20	x	[28]
$LiF-LiI_2$	83.5:16.5	50.00	3.68	x	[28]
$LiF-NaF-ZrF_4$	55:22:23	20.45	2.72	x	[28]
$LiCl-BeCl_2$	1:1	20.00	–	x	[29]
$LiCl-PbCl_2$	1:2	12.50	4.50	x	[29]
$LiCl-KCl$	7:3	35.00	1.60	x	[29]
$LiCl-KCl$*	52:48	26.00	1.60	x	[29]
$LiCl-NaCl$	72:28	36.00	1.60	x	[29]

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