European Master of Science
in Nuclear Fusion and Engineering Physics

# Nuclear Analysis for a Magnetic Fusion Reactor

Master Thesis
presented by

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# Abstract

This work describes neutronics modelling of a one dimensional generic magnetic fusion reactor using the OpenMC code. The geometry of the discussed models include a simple model of the blanket, the vacuum vessel and the magnets. The blanket includes options for tritium breeding and shielding depending on whether D-T or D-D fusion is pursued as the primary fusion reaction. In the case of tritium breeding, pure natural liquid lithium has been considered. In the case of shielding, magnesium borohydride is used. The thickness of the these layers is varied to derive optimal dimensions for breeding, targeting a tritium breeding ratio in the range 1.1 to 1.2, and for shielding, targeting coil heating levels below or equal to 2.32e-05 eV/source-neutron . The analysis indicates that in the case of D-D fusion, breeding blanket of liquid lithium is not required and a magnesium borohydride shield thickness of 55 cm and 20 cm for the cases mentioned in sections 3.7.1 and 3.7.2 respectively are optimal.

# Contents

# Chapter 1

# Introduction

This purpose of this Chapter is to introduce the readers with the basic idea about the need of nuclear energy, the types of phenomena involved, the nuclear reactions involved in them and their contribution and utilisation in curbing out the present day energy crisis around the globe.

## 1.1 Energy Demand vs Crisis/Choice

Until date, living beings have witnessed various wars and battles and were successful in fighting back. The positive side of such conflicts were/are visible. But the one which gets ignored is the environmental warfare. In this smart twenty first century, the major global issue is global warming, occurring due to climate change. It is true that the change in climate can be natural until a certain level but is hugely impacted by human activities. The primary activity includes usage and burning of fossil fuels, the natural source of fuel/energy on earth, the repository of which will be empty soon in future which might lead to a energy-less globe. This might sound catastrophic but if alternative source of energies are not being adapted, this nightmare would turn out to be true.

It is clearly evident from the heading of this section that the battle is not between the demand and crisis of energy, rather it is between the demand and the choice of energy resource.

Moreover, another major consequence of fossil fuel burning is environmental pollution. We are very familiar with the very known impact of pollution, the Ozone Layer Depletion. Due to this depletion, the level of ultra violet (UV) radiation on earth has been increased. This has given immense stress to the environmentalists due to the harmful and hazardous impact of UV radiation on human health leading to diseases like skin cancer.

Energy demand has already been skyrocketed and it will increase in the near future under the combined pressure of population growth, urbanization and expanding access to energy. Hence as it is next to impossible to suppress the energy demand, it is advisable and recommended to seek and opt for alternative as well as sustainable resource of energy.

The sectors of alternative energies include, solar energy, wind energy, hydro power (energy extracted from water), geothermal energy and the very efficient nuclear energy.

## 1.2 Nuclear Energy

Nuclear energy is a form of energy which is produced from the nucleus, or core of an atom. It is well-known to us that atoms are tiny units that make up all matter in the universe, and the energy which binds the nucleus together is known as binding energy. There is a huge amount of energy in an atom's dense nucleus. In fact, the force that holds the nucleus together is known as the "strong force."

In the process of a nuclear reaction, two nuclei, or a nucleus and an external subatomic particle, collide to produce one or more new nuclides. Thus, a nuclear reaction must cause a transformation of at least one nuclide to another.

If a nucleus interacts with another nucleus or particle and then they separate without changing the nature of any nuclide, then the process is simply referred to as a type of nuclear scattering, but not a nuclear reaction. A nuclear reaction can either be endothermic or exothermic in nature depending on the mass of the nuclide.

In nature, nuclear reactions occur in the as an interaction between cosmic rays and matter.

The two general types of nuclear reactions are [1] :

- Nuclear Decay: In case of nuclear decay, an element that with an unstable nucleus emits radiation and gets transformed into the nucleus of one or more other elements of stable kind or followed by successive decays if the product of the initial decay is also unstable. The resulting daughter nuclei have a lower mass and are lower in energy (more stable) than the parent nucleus that decayed. Nuclear decay reactions can occur spontaneously under all conditions provided the nucleus of the parent element is unstable.

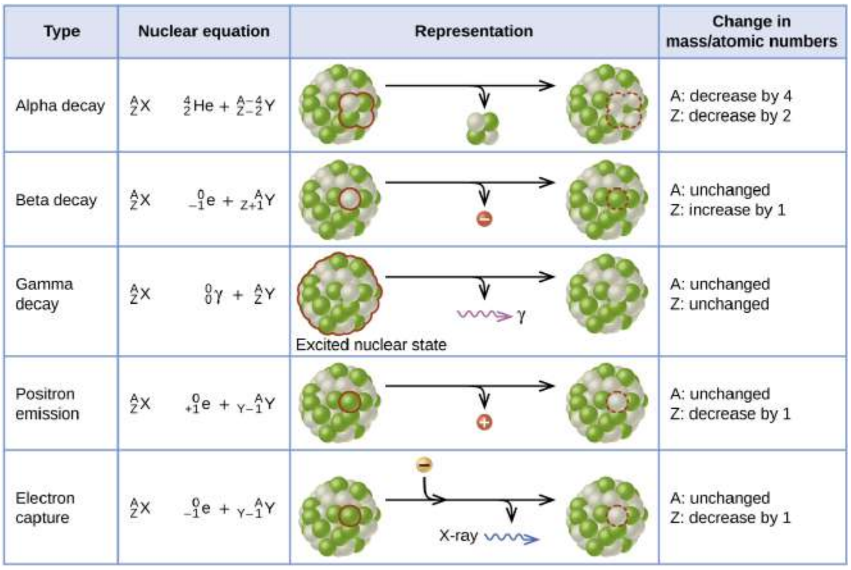


*Figure 1.1: Various modes of Nuclear Decay [2]*

- Nuclear Transmutation: In the process of nuclear transmutation a nucleus reacts with a subatomic particle or another nucleus to form a product nucleus that is more massive than the initial one. Unlike nuclear decay, nuclear transmutation reactions occur only under very specific conditions, such as the collision of a beam of highly energetic particles with a target nucleus or in the interior of stars. Nuclear transmutation reactions are basically the induced ones. The first successful nuclear transmutation reaction was carried out in 1919 by Ernest Rutherford, who showed that particles emitted by radium could react with nitrogen nuclei to form oxygen nuclei. As shown in the following reaction, a proton is emitted in the process: ${}^{4}_{2}\alpha^{+}\, {}^{14}_{7}\mathrm{N} \longrightarrow {}^{17}\mathrm{O}_{8} + {}^{1}_{1}\mathrm{p}$ This is an alpha particle-induced nuclear reaction.

Nuclear energy can efficiently be used to produce energy which can be further used to generate power and electricity.

The two branch of nuclear phenomena that can be used to produce energy are:

- Nuclear Fission
- Nuclear Fusion

Nuclear chain reactions in fissionable materials produce induced nuclear fission. Various nuclear fusion reactions of light elements power the energy production of the Sun and stars. Nuclear power has a vital role to play in helping to address the global climate emergency.

Now, let's speculate the two major domains of nuclear reactions which can play a vital role in curbing energy crisis with zero carbon emission.

## 1.2.1 Nuclear Fission - the existing choice

The phenomenon of nuclear fission was discovered in December 1938 by chemists Otto Hahn and Fritz Strassmann and physicists Lise Meitner and Otto Robert Frisch.

This phenomenon involves splitting of the nucleus of an atom into smaller nuclei. This reaction usually produces gamma photons and releases a significant amount of energy. This output energy is even high for radioactive decay standards. The present-day nuclear power plants are based on the nuclear fission phenomenon.

### 1.2.1.1 How does nuclear fission reactor work? [3]

Nuclear power refers to the generation of electricity by harnessing the controlled release of nuclear energy, the force that binds atomic nuclei together at the core of atoms. These nuclei serve as the central components of atoms. Through the process of nuclear fission, wherein the nuclei of particular materials split, nuclear energy is ultimately released, typically in the form of heat. Uranium, a naturally occurring weakly radioactive heavy metal abundant in the Earth's crust, is the predominant material used in nuclear fission. Typically, uranium is loaded into fuel rods, frequently following the enrichment process to enhance its ability to undergo fission. Subsequently, these rods are placed inside the nuclear reactor.

In pressurized water reactors, which are the prevailing type of nuclear power reactors employed globally, the fuel rods are positioned within the reactor's vessel, which is filled with water. Within this setup, the fuel rods are subjected to a bombardment of nuclear particles known as neutrons, initially produced by a neutron source device located inside the reactor. As a result, the uranium nuclei in the fuel rods undergo splitting, resulting in the release of energy and additional neutrons. These newly released neutrons then induce the splitting of other uranium nuclei within the fuel rods, continuing the chain reaction of nuclear fission.

Within pressurized water reactors, the energy liberated during nuclear fission results in the elevation of temperature in both the fuel rods and the encompassing water. To avoid boiling, the water is maintained under pressure, while the generated heat is transferred to a separate vessel where it is employed to boil water. This boiling water generates steam, which in turn drives a large turbine at high velocities. Connected to this turbine is a generator that spins, converting the mechanical energy into electrical energy. Subsequently, the produced electricity is transmitted through a power grid, which serves as a network for distributing electricity from producers to consumers.

The process of nuclear fission persists until control rods, typically composed of neutron-absorbing materials like cadmium, are introduced between the fuel rods. These control rods effectively halt the chain reaction of nuclear fission by absorbing neutrons without triggering further fissions.

Here's an example of nuclear reaction in producing energy using ${}^{235}_{92}\mathrm{U}$ as fuel:

${}^{1}_{0}\mathrm{n} + {}^{235}_{92}\mathrm{U} \longrightarrow {}^{236}_{92}\mathrm{U} \longrightarrow {}^{92}_{36}\mathrm{Kr} + {}^{141}_{56}\mathrm{Ba} + 3\,{}^{0}_{1}\mathrm{n} + \mathrm{Energy}$

### 1.2.2 Nuclear Fusion -a pathway to a cleaner energy

In nuclear fusion, two different heavier isotopes of hydrogen — deuterium and tritium are fused to produce one helium atom and a very high energetic neutron ( 14MeV). Harnessing this released energy in an efficient way will result in controlled nuclear fusion.

It is by this process our own natural power reserve, "The Sun" charges itself and provides the world with rays of light. In the Sun, two protons (1H) undergo a simultaneous fusion and beta decay to form a positron($\mathrm{e}^{+}$), a neutrino ($\nu$) and a deuteron ($\mathrm{D\,or\,{}^{2}H}$). The deuterium nucleus, called deuteron contains one proton and one neutron.

$$\mathrm{p} + \mathrm{p} \longrightarrow \mathrm{D} + \mathrm{e}^{+} + \nu$$

Two gamma rays are released as a result of annihilation of the positron with a free electron from the environment.

The deuteron reacts with another proton resulting in a Helium nucleus (${}^{3}_{2}He$ i.e. an isotope of helium with two protons and one neutron) and a gamma ray.

$$\mathrm{D} + \mathrm{p} \longrightarrow {}^{3}_{2}\mathrm{He} + \gamma$$

A ${}^{4}_{2}He$ nucleus and two protons are formed as a result of fusion of two ${}^{3}_{2}He$ nuclei produced in two separate events. Again, these two protons undergo a simultaneous fusion reaction followed by beta decay and the cycle continues. This reaction cycle is termed as the proton-proton (p-p) cycle. Thus it can be concluded that hydrogen is being converted to helium through p-p cycle.

Whereas in comparatively heavier stars, the CNO (carbon-nitrogen-oxygen) cycle dominates the p-p cycle. It is also known as Bethe–Weizsäcker cycle.

Now, it is our objective and responsibility to imitate and adopt this sustainable zero-carbon emitting option as a the resource for global energy supply.

The basic requirements for successful operation of a thermonuclear reactor are:

i. a high particle density

ii. a high plasma temperature (plasma is the fourth state of matter, necessary to bring two positive ions together)

iii. a long confinement time inside the reactor.

The proton-proton (p-p) cycle is quite impossible for use in a terrestrial fusion reaction as the initial step is an extremely slow process, taking a billion years.

The most acceptable terrestrial-based fusion reactions are :

i. D-D Reaction

where, D is Deuterium ($^2_1H$), the second isotope of Hydrogen). This reaction has two possibilities with :

A. $^2_1\mathrm{H} + ^2_1\mathrm{H} \longrightarrow ^3_2\mathrm{He} + ^1_0\mathrm{n}(2.45\,\mathrm{MeV})$

Two deuterium nuclei fused to form a $^3He$ nucleus and a free neutron.

B. $^2_1\mathrm{H} + ^2_1\mathrm{H} \longrightarrow ^3_1\mathrm{H} + ^1_1\mathrm{p}$

Two deuterium nuclei fused to produce a Tritium and a high-energy proton.

ii. D-T Reaction where, T is Tritium ($^3_1H$), the third isotope of Hydrogen.

A. $^2_1\mathrm{H} + ^3_1\mathrm{H} \longrightarrow ^4_2\mathrm{He}(3.5\,\mathrm{MeV}) + ^1_0\mathrm{n}(14.1\,\mathrm{MeV})$

A deuterium nucleus and a tritium nucleus fuses to produce an alpha particle and a free 14.1 MeV neutron. Due to large energy release, D-T reaction is chosen to be used in controlled fusion reactors.

Among the above mentioned two types of fusion reaction, usually D-T reaction is chosen over the D-D fusion reactions for building a model fusion reactor device because of high reaction cross-section of the former one.

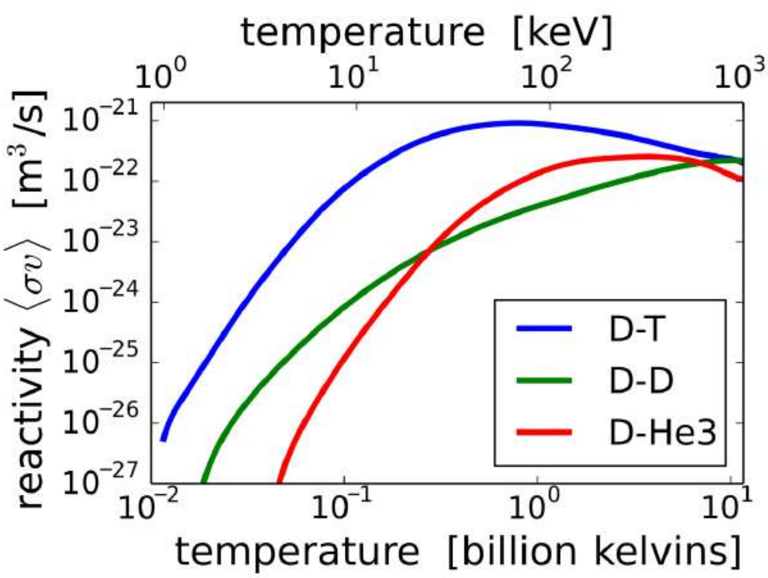


*Figure 1.2: Reaction Cross-section of Fusion Reactions [4]*

#### 1.2.2.1 Why switching from Fission to Fusion? [5]

To drive Nuclear Fission, the reaction components require radioactive elements such as Uranium. It might be an issue for nations who don't have an adequate amount of Uranium reserve.

Although, nations like India who has Thorium reserves have adopted for a Thorium-based nuclear power program.

- Abundant energy: Controlled fusion reaction unleashes energy that is nearly four million times more powerful than energy released from chemical reactions such as burning coal, oil, or gas. It also surpasses nuclear fission reactions by fourfold in terms of energy output per unit mass. The potential of fusion lies in its capacity to provide a stable and abundant source of energy, capable of meeting the electricity demands of our cities and industries.
- Millions of years: To achieve fusion in a reactor, two elements—deuterium and tritium—are necessary. Deuterium can be extracted from various water sources, while tritium is produced during the fusion reaction through the interaction of fusion neutrons with lithium. The presence of lithium reserves on Earth would enable the operation of fusion power plants for over 1,000 years, and utilizing sea-based lithium reserves in the form of Li-6 isotope could fulfill the energy needs for millions of years. However, a crucial hurdle involves the dependable breeding and recovery of tritium within a fusion device.
- Zero CO Emission: Fusion does not release harmful substances such as carbon dioxide or other greenhouse gases into the atmosphere. Instead, its primary by-product is helium, which is an inert and non-toxic gas.
- No trace of long-lived radioactive waste: Nuclear fusion reactors do not generate highly active, long-lived nuclear waste. In contrast, nuclear power plants that operate on fission reactions produce waste with varying degrees of radioactivity, which are managed according to their levels of radioactivity and intended purpose. The activation of components in a fusion reactor is projected to be sufficiently low, allowing for the recycling or reuse of materials within a span of 100 years. The duration may vary depending on the specific materials utilized in the "first-wall" that faces the plasma.
- Limited risk of proliferation:Fusion does not utilize fissile materials such as uranium and plutonium. It is important to note that radioactive tritium, although present in fusion reactions, is neither fissile nor fissionable. In a fusion reactor like ITER, there are no enriched materials that could be exploited for the production of nuclear weapons.
- No risk of meltdown: The occurrence of a Fukushima-like nuclear accident is not feasible in a tokamak fusion device. Achieving and sustaining the precise conditions required for fusion is already challenging, and any disruption results in rapid cooling of the plasma and the cessation of the reaction. The amount of fuel present in the vessel at any given time is only sufficient for a few seconds, eliminating the risk of a chain reaction.

### 1.2.3 What are the benefits of nuclear energy? [6]

- In contrast to several renewable energy sources, nuclear energy has the advantage of being capable of continuous power generation, unaffected by weather conditions such as those impacting wind and solar power.
- This consistent availability of nuclear power enables it to meet energy demands more reliably, thereby reducing the carbon intensity of the electricity supply during periods when other renewable sources may be less accessible.
- Furthermore, certain advanced nuclear power plants are now authorized to operate for up to 80 years, surpassing the lifespan of gas, coal-fired power stations, and many renewable

energy installations. However, it is important to consider various significant expenses associated with nuclear power. These include upfront costs, decommissioning expenses, and the costs of storing depleted fuel and other materials. Additionally, nuclear power plants require extensive maintenance throughout their operational lifespan.

#### 1.2.3.1 Clean Source of Energy [6]

- Nuclear power is recognized for its low emissions profile. It is categorized as a clean energy source since it generates no carbon emissions or other harmful greenhouse gases during its operation.

- Additionally, when considering the complete life cycle of nuclear energy, including all stages of production, its emissions are substantially lower than those associated with fossil fuel-based electricity generation.

#### 1.2.3.2 Renewability [6]

Nuclear fuels, like uranium, are classified as non-renewable resources because they are finite materials extracted from specific locations. Nevertheless, nuclear power stations utilize a minimal amount of fuel to generate the same electricity output as coal or gas power stations (1 kg of uranium equals 2.7 million kg of coal), making them a reliable energy source for many decades to come. Concerns arise regarding the management of spent fuel from reactors, as there is still no definitive and risk-free method for its long-term disposal. However, despite the need to keep decommissioned nuclear sites and their structures untouched for significant periods of time, it is possible to construct a new reactor on the same site. Spent Fuel reprocessing is an important step involved in the existing nuclear power program

#### 1.2.3.3 How much is nuclear energy currently used? [7]

- During 1950s, the first commercial nuclear power stations started to operate.

- About 10% of world's electricity is being contributed by nuclear energy and this portion is being produced by 440 power reactors.

- Nuclear is the world's second largest source of low-carbon power (26% of the total in 2020).

- Over 50 countries utilize nuclear energy in about 220 research reactors.

- In addition to research, these reactors are used for the production of medical and industrial isotopes, as well as for training.

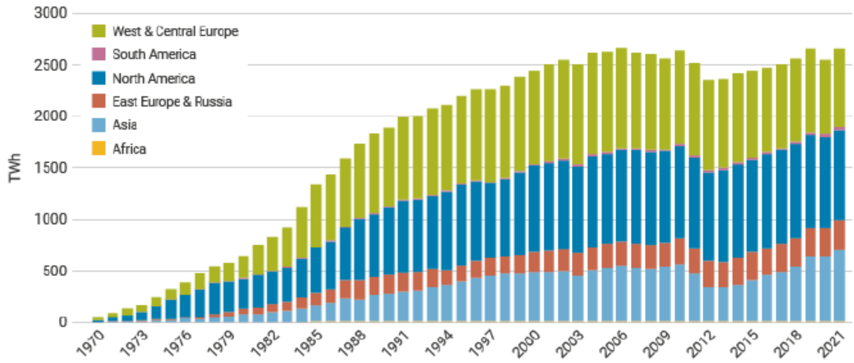


*Figure 1.3: Nuclear electricity production(source: World Nuclear Association, IAEA PRIS [7]*

### 1.2.4 Futuristic version- Small Modular Reactors(SMRs)

The future may also see the introduction of Small Modular Reactors (SMRs). These are smaller version of nuclear power plants, similar to those that power nuclear submarines and ships. While SMRs' power output is substantially less than a full-scale nuclear power station (they generate as little as a fifth of current-generation reactors), they can be more easily manufactured and transported to where they're needed, before being dismantled and returned at the end of their operating life.

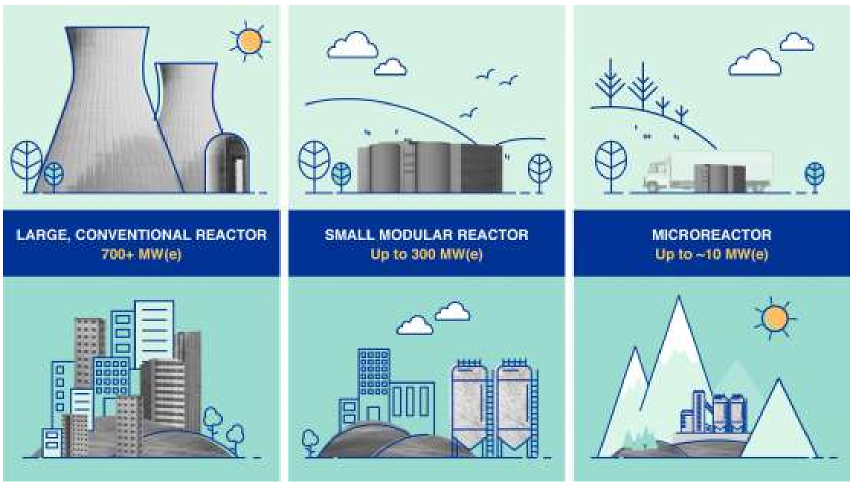


*Figure 1.4: Comparative idea of an SMR [8]*

# Chapter 2

# Concept of Breeding

This chapter is dedicated to discuss the concept and purpose of Tritium Breeding.

## 2.1 Purpose of Breeding

As discussed in section 1.2.2 tritium (T) and deuterium (D) are the two key components (isotopes of hydrogen) that will be used to drive the fusion reaction and help the fusion reactor operate. While deuterium can be extracted from seawater in virtually boundless quantities, the supply of available tritium is limited, estimated currently at twenty kilos.

Deuterium can be distilled from all forms of water. It is a widely available, harmless, and virtually inexhaustible resource. In every cubic metre of seawater, for example, there are 33 grams of deuterium. Deuterium is routinely produced for scientific and industrial applications.

Tritium is a fast-decaying radioactive element of hydrogen which occurs only in trace quantities in nature with a half-life of 12.3 years. It can be produced during the fusion reaction through contact with lithium, however: tritium is produced, or "bred," when neutrons escaping the plasma interact with lithium contained in the blanket wall of the tokamak.

Lithium from proven, easily extractable land-based resources would provide a stock sufficient to operate fusion power plants for more than 1,000 years. What's more, lithium can be extracted from ocean water, where reserves are practically unlimited (enough to fulfill the world's energy needs for   6 million years).

### 2.1.1 Tritium Breeding Mechanism

Among the types of fusion reaction in 1.2.2, the D-T reaction is considered over the D-D reaction. The reason being higher cross-section of the D-T reaction and a larger Q-value. In a fusion reaction,it is very necessary for the reactants to overcome the Coulomb barrier with the aid of tunneling.

$$TBR = \frac{\textit{Number of Tritium Produced per unit time}}{\textit{Number of Tritium Consumed per unit time}} \tag{2.1}$$

In the deuterium-tritium (D-T) fusion reaction, high energy neutrons are released along with helium atoms. These electrically-neutral particles escape the magnetic fields that confine the plasma and are absorbed by the blanket covering the surrounding walls.

If the blanket modules contain lithium, a reaction occurs: the incoming neutron is absorbed by the lithium atom, which recombines into an atom of tritium and an atom of helium. Then tritium can be extracted from the blanket and recycled into the plasma as fuel.

Blankets containing lithium are referred to as breeding blankets. Through them, tritium can be bred indefinitely. Once the fusion reaction is established in a tokamak, deuterium and lithium are the external fuels required to sustain it. Both of these fuels are readily available.

Steps involved in the reaction mechanism of Tritium Breeding:

- ${}^{2}_{1}\mathrm{H} + {}^{3}_{1}\mathrm{H} \longrightarrow {}^{4}_{2}\mathrm{He} + {}^{1}_{0}\mathrm{n}$

The neutron produced in the above mentioned D-T reaction is of very high energy (14.1 MeV). This 14.1 MeV neutron after undergoing an neutron-induced reaction with ${}^{6}Li$ or ${}^{7}Li$ will produce tritium.

- ${}^{6}_{3}\mathrm{Li} + {}^{1}_{0}\mathrm{n} \longrightarrow {}^{3}_{1}\mathrm{T} + {}^{4}_{2}\mathrm{He}$
- ${}^{7}_{3}\mathrm{Li} + {}^{1}_{0}\mathrm{n} \longrightarrow {}^{3}_{1}\mathrm{T} + {}^{4}_{2}\mathrm{He} + {}^{1}_{0}\mathrm{n}$

Tritium Breeding Ratio (TBR) is the ratio of the rate of tritium bred in the blanket to the rate tritium burnt in the plasma. It is very much necessary to build a self-sufficient fusion device, the reason behind the lack of natural resource of tritium. Hence, a key part of the most of the proposed fusion reactor devices is the Tritium Breeding Blanket.

### 2.1.2 Self-Sufficiency Criterion [9]

Since Tritium is playing a crucial role in the development and operation of D-T fusion plants, it is necessary to generate tritium in sufficient quantities as well as extract it efficiently to ensure tritium self-sufficiency. But the transport and permeation of tritium generated and extracted needs to be controlled since Tritium is radioactive and hence it is a safety and biological hazard.

The tritium self-sufficiency criterion can be defined as:

$$TBR_a > TBR_r \tag{2.2}$$

where $TBR_a$: achievable tritium breeding ratio $TBR_r$: is the required tritium breeding ratio Both of the above-mentioned parameters are complex functions of plasma physics, materials, and technology choices and operating parameters.

The required TBR must exceed unity by a margin to:

1. Compensate for losses and radioactive decay (5.47% per year) of tritium between production and use.
2. Supply tritium inventory for start-up of other reactors (for a specified doubling time).
3. Provide a "reserve" storage inventory necessary for continued reactor operation under certain conditions (e.g. a failure in a tritium processing line).

A dynamic model was developed by Mr. Mohammed Abdou et al. to calculate time-dependent tritium flow rates and inventories and to accurately determine required TBR.

### 2.1.3 Functionalities of Tritium Breeding Blanket

The purpose of the breeding blanket is not limited to breed tritium. Besides, the breeding blanket also serves the following:

1. It also absorbs the energy released from neutrons produced within the plasma as a result of the fusion reactions which enhances the cooling mechanism and maintains the temperature within the reactor vessel.

2. In addition, the breeding blanket also serves the purpose of a shield by keeping the high energy neutrons contained with the reactor vessel area, so that they don't escape to the other more radiation-susceptible regions such as ohmic or superconducting magnets and protect them from damage.

The breeding blanket will guarantee a self-sustaining tritium loop for reactor fueling.

### 2.1.4 Desirable properties of Breeding Blanket Materials

- Withstand high mechanical and thermal loads

- Should not tend to become radioactive upon completion of their useful service life.

### 2.1.5 Concepts of Breeder Blanket

Breeding blanket designs are mostly based on lithium containing ceramics such as lithium titanate [(Mixed oxide(lithium, titanium, oxygen)], lithium orthosilicate($\mathrm{Li_4SiO_4}$). Lithium Titatnate is used in pebble form to produce and extract tritium and helium. Various types of breeder blanket are as follows:

- Helium-Cooled Lithium Lead(HCLL)

- Helium-cooled pebble bed(HCPB)

- Water-cooled lithium lead(WCLL)

In the first ever nuclear fusion reactor, ITER(International Thermonuclear Experimental Reactor), 6 different types of tritium breeding systems, knows as Test Blanket Modules(TBM) will be tested.

### 2.1.6 Why $^6Li$ over $^7Li$ ?

- High abundance of $^6Li$.

- Neutron-induced reaction with $^7Li$ is less likely to occur.

Now, it's time to build a model of prototype fusion reactor device with a tritium breeding concept using liquid breeder material. The model will be beneficial and provide an idea of tritium production.

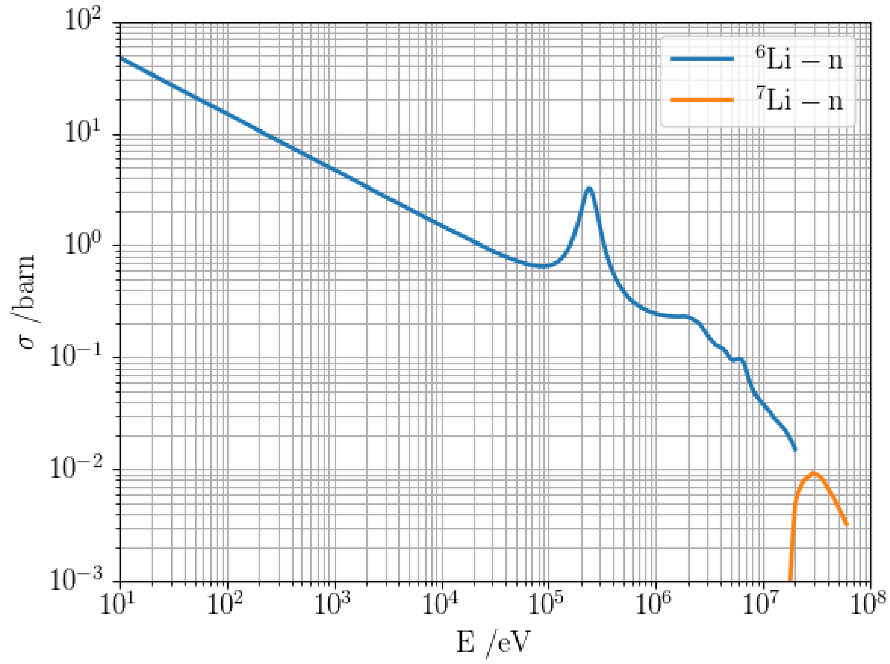


*Figure 2.1: Cross-section for neutron-induced reaction of* $^6Li$ *and* $^7Li$. *[10]*

# Chapter 3

# Approach to the Objective

This Chapter is dedicated to discuss the objective of this study and approach that has been followed to fulfil the concept of a magnetically confined fusion reactor device with a liquid breeding blanket.

## 3.1 Objective

The purpose of this study is to identify optimal dimensions of lithium breeding material and neutron shielding for a DT burning fusion magnetic fusion reactor. The key metrics are the tritium breeding ratio TBR (tritium atoms produced per thermonuclear neutron) and heat deposition in an assumed magnet coil. The achieved TBR required be above 1 to ensure sufficient tritium replacement in the face of tritium loss via diffusion into the fusion reactor materials. The heat deposition in the coils, which are assumed to be cryogenically-cooled, should be minimized to reduce the capital cost of the refrigeration plant and its operating cost, the latter impacting the required recirculating power in the fusion plant. For comparison with the DT burning case, a magnetic fusion reactor based on DD fusion is also considered. In this case, no tritium breeding is required and the neutron spectrum has a component at lower energy (i.e. 2.45 MeV, compared to the DT-generated neutron at 14.1 MeV). A Monte Carlo method is most suited for this type of neutron transport and reaction calculation. Several existing codes exist in this domain. It was decided to use the OpenMC code, as it is readily available, open source and used extensively in magnetic fusion development.

## 3.2 Magnetic Fusion Reactor

In this task a magnetic fusion reactor has been considered for the analysis. It is already known that for a consistent fusion reaction it is very much essential to confine plasma for a longer time. And this confinement is done by virtue of the magnetic field lines. Hence, it is said that the plasma is magnetically confined .

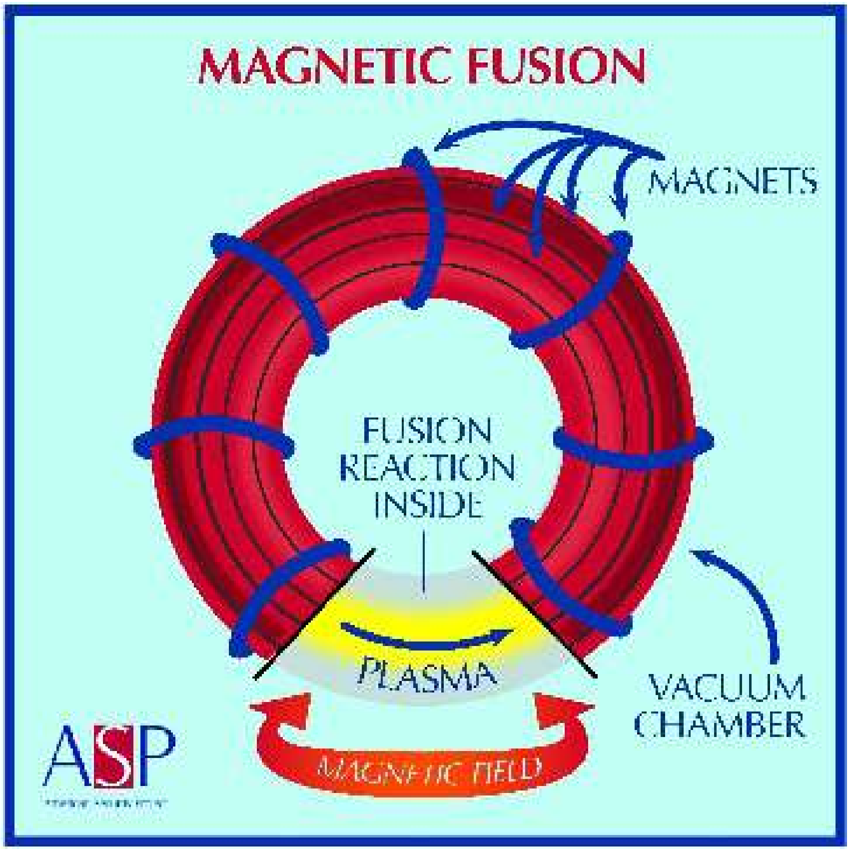


*Figure 3.1: Concept of Magnetically Confined Fusion [11]*

## 3.3 Geometry of the discussed models

In this project,the geometries of the discussed models are cylindrical in shape instead of a D-shaped or a toroidal symmetrical vacuum vessel concept. The main reason behind choosing this geometry is to build a simplified model with faster simulations and calculations. The D-shaped model would definitely allow the neutrons to travel longer distances than in cylindrical geometry but that would not impact the Tritium Breeding Ratio (TBR). This approximation of cylindrical geometries works well in case of systems with larger aspect ratio, A [ where, A = MajorRadius(R)/MinorRadius(a)].

The initial geometry consists of the vacuum vessel, followed by the first wall material, breeding blanket, shield material, structural material and the conducting coil. The latter two geometries are modified versions of the former one.

To fulfil the objective, three scenarios have been taken into consideration and they are as follows:

- D-T Model (14.1 MeV neutron Source)- The purpose of this model is to decide the required thickness of the liquid breeder blanket material which would fulfill the self-sufficiency criterion as well as the required shield thickness so that least amount of heat is deposited in the coils and least number of neutrons can escape and neutron-irradiation damage can be avoided.
- D-D Model case 1 (14.1 MeV neutron Source)- The basic principle of this model is the release of a 14.1 MeV neutrons as a result of an induced D-T fusion reaction which can

occur between the deuterium reactant from the D-D reaction and the Tritium product from one of the mentioned branches of D-D reaction. The purpose of this model is to check and decide the thickness of shield material in order to shield the fast neutrons so that the leakage fraction is the least.

- D-D Model case 2 (2.45 MeV neutron Source)- The basic principle of this model is based on that particular branch of D-D reaction which releases a neutron of 2.45 MeV, so that the required thickness of the shield material to moderate 2.45 MeV neutrons can be decided.

In all of the three scenarios, the geometry of each model remains cylindrical whereas the thickness of the material layers have been varied as per requirement to achieve the optimal values.

The dimensions of the vacuum vessel remains same in all three models. It has a radius of 110 cm. The height of the entire cylindrical geometry including the vacuum cylinder in the centre is 100 cm. The upper and lower surface is common for the of the entire cylindrical geometry with boundary type set to 'reflective'. The boundary type of the rest of the shared surfaces are by default transmissive (so that particles can freely pass through surfaces) except that of the last layer (the copper layer). The boundary type of the copper layer is set to 'vacuum'.

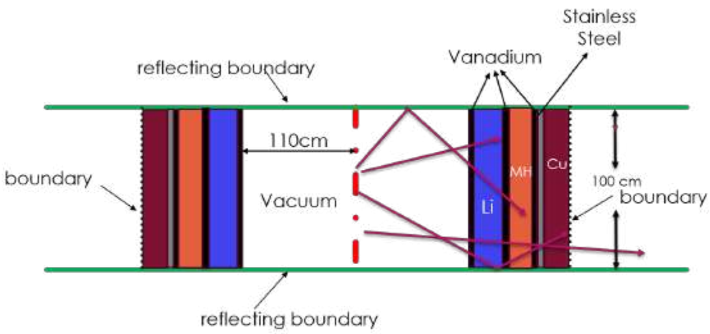


*Figure 3.2: A generalised schematic of the discussed models with the boundary types labelled.*

## 3.4 Idea behind the modelling

As already mentioned, the toroidal geometry has been approximated by using a cylindrical geometry to narrow it down to a one-dimensional problem.

Considering the following assumptions:

- $R_0$ (Major Radius of Magnetic Fusion device) = 5m =500cm
- $P_{fus}(FusionPower) = 618MW$
- $P_{th}(\ldots + P_{alpha}) = 667MW$
- $P_{neutrons} = 494MW$
- Energy of each fast neutron = 14.1 $MeV$

Calculating the neutron flux based on the above assumptions:

Neutron flux = $494MW/(14.1MeV$*1.6*$10^{-19}J/eV)$ ≈2.19*$10^{20}n/s$

Hence, Neutron Flux Density = Neutron Flux/Area of Torus

Area of Torus = (2*pi*R0)(2*pi*a) (assuming a= 109 cm as in case of the models discussed below)

Where, a: Minor Radius of the magnetic fusion device

Therefore, Neutron Flux Density ≈1.02 * $10^{14} cm^2$

Assuming, the cross-section of the copper coils as 20cm*20cm (as considered the radius of the copper layer in the discussed models). The coils in a tokamak or stellarators are discrete and instead of covering the entire periphery, they cover only 10% of the periphery and hence absorbs only 10 % of the neutrons that reach this radius.

Considering, Number of Conducting Coils = 16

Therefore fraction intercepted by coil = 16 *20cm/(2*pi*500) = 0.10 = 10%

Assuming, the amount of neutron power is 73kW i.e 0.073 MW at cryogenic temperature of 20K.

Using Reversed Carnot Cycle (Refrigeration), calculating the required amount of work to be done to bring the neutron power of 0.73 MW from 293 K to 20 K:

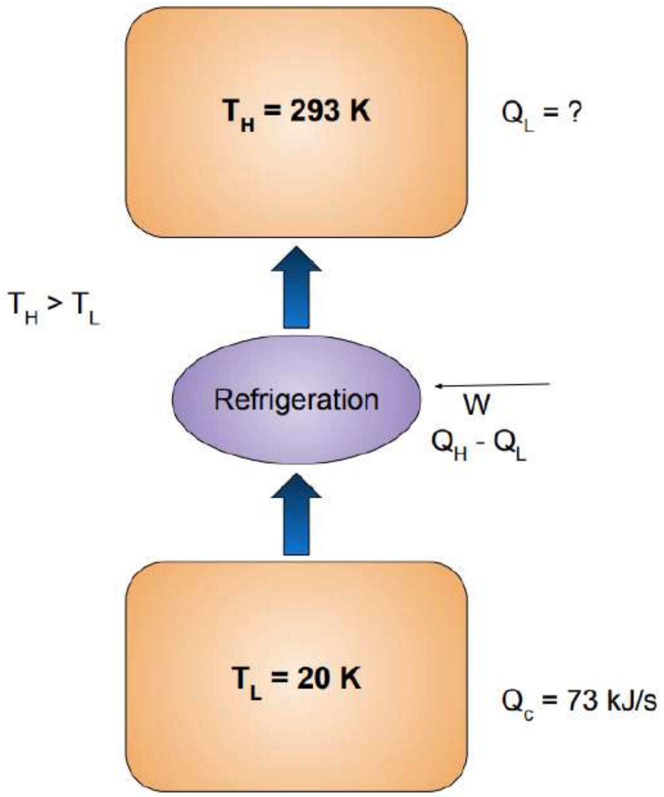


*Figure 3.3: Schematic of Reversed Carnot Cycle*

Coefficient of Performance:

$$\frac{Q_c}{W} = \frac{T_c}{T_h - T_c} \tag{3.1}$$

Therefore, $\frac{Q_c}{W} = 0.073$

And hence, $W = 10^3 kJ/s = 1MW$

It has been calculated and found that a work of 1 MW needs to be done to bring back this neutron power to 293 K from 20 K. Hence, this implies that cooling down a neutron power of 73kW from 293 K to cryogenic temperature of 20 K to maintain the superconductivity is 1 MW. This gives an idea how important it is to have least energy deposition in coils and avoid overheating of coils.

73 kW in the discrete magnets would be the equivalent to 10 x 73 kW in the 1 D model.

Power in Magnet(Assuming Copper Coils) will be:

Neutron Power at Cryogenic Temperature/ Fraction intercepted by Coils $= \frac{0.073MW}{0.10} = 0.73MW$

Ratio: (Power in Magnet/Neutron Power(assumed)) $= \frac{0.73MW}{494MW} \approx$ 1.5* $10^3$ of the total neutron power.

## 3.5 Materials used in the discussed models

The materials used in the mentioned models has been discussed below:

### 3.5.1 Lithium

In the discussed models, pure natural liquid lithium(mixture of $^6Li$ and $^7Li$ has been used as a breeding material to breed tritium by virtue of the neutron-induced reactions as mentioned in section 2.1.1 within the reactor vessel and build it as a self-sufficient one.

| **Property** | **Value/Composition** |
|---|---|
| *Density* | 0.49 g/cm³ (at 900 K) |
| *Name of Nuclide* | |
| Lithium-6 (Li-6) | 7.4 atom percent (ao) |
| Lithium-7 (Li-7) | 92.6 ao |

*Table 3.1: Specification of Breeding Material*

As we are considering a liquid breeding blanket, liquid lithium has been used to breed tritium and build a self-sustaining fusion reactor device.

#### 3.5.1.1 But why liquid breeder?

Liquid lithium/vanadium (Li/V) self-cooled blanket concept has many advantages over solid breeder blanket such as:

- simple structure
- high thermal efficiency due to operation at high temperature
- low after-heat
- good tritium breeding capability

### 3.5.2 $\mathrm{V}{-}4\,\mathrm{Cr}{-}4\,\mathrm{Ti}$ Alloy [12]

The purpose of using this vanadium alloy is because it has been identified as an ideal material to be used for first-wall material or for blanket applications in fusion reactor devices.

There are certain vanadium alloys which has the following favorable safety characteristics:

- Good fabricability.
- Capability to sustain High Temperature and Heat Load.
- Good compatibility with liquid metal coolants.
- High Resistant to neutron-irradiation damage.

Due to high thermal stress factor, sustainability to high temperature and low activation property, vanadium alloys are recognized as ideal material for neutron interactive structural components to be used in fusion devices.

The characteristic high compatibility of vanadium alloys with liquid lithium makes it possible to design concepts of liquid Li blanket using vanadium alloys, which have the potential of high thermodynamic efficiency, high reliability and availability because of high operation temperature and no need for neutron multiplier and ceramic breeder, both of which must be replaced periodically owing to burn-up.

The ternary alloys of V-Cr-Ti and V-Ti-Si are being evaluated for use in fusion reactors for the first wall and blanket structure. Pure vanadium must be used to produce these alloys and may be important in producing other vanadium-containing alloys with improved properties.

Low long-term activation is a property of vanadium, chromium, titanium and silicon. Under a high flux of neutrons, radioisotopes of vanadium, chromium and titanium are formed in the alloy. These radioisotopes have short half-lives which result in rapid radioactive decay. This short decay-time allows for safer disposal than is possible with alloys containing many other elements.

Vanadium has a low fusion-neutron cross section, and its inelastic-scattering cross section is also quite small. These favorable nuclear properties, coupled with vanadium's high melting point, ductility, and good physical properties, make the metal of particular interest as a structural material for fast reactors. Favorable alloying characteristics with uranium also make the metal of interest as a diluent, although the transport cross section is small. The thermal neutron cross section of vanadium is large, however, and its usefulness in thermal reactors is limited.

In this geometrical design, vanadium alloy layers depict the walls of the vanadium-alloy containers in which the breeding material (liquid lithium) as well as the shield material is being sealed. It serves as a good structural materials in presence of high energetic neutrons.

| **Properties of Vanadium Alloy** | **Value/Composition** |
|---|---|
| *Density* | 6.05 g/cm³ |
| *Name of Element* | |
| Vanadium | 92.5 weight percent (wo) |
| Chromium | 4.12 wo |
| Titanium | 4.13 wo |

*Table 3.2: Specification of Vanadium Alloy ( $\mathrm{V{-}4\,Cr{-}4\,Ti}$ ) [12]*

### 3.5.3 Magnesium Borohydride

The compound $\mathrm{Mg(BH_4)_2}$ (Magnesium Borohydride) has been used as a shield material.

The hydrogen-rich hydrides show superior neutron shielding capability compared to the conventional materials. In general, a hydrogen-rich material has the potential to be an effective neutron shield because the contained hydrogen nuclei work as a moderator of fast neutrons, reducing the fast neutron flux. This indicates that neutron shielding capability depends heavily on the hydrogen concentration. [13]

Magnesium borohydride is a desirable choice and has attracted considerable attention for its extremely high hydrogen capacity (14.9 wt% by mass and 145–147 kg $cm^-3$ by volume). [14]

The composition percentages of magnesium borohydride has automatically been added via OpenMC as this material has been added via the chemical formula unlike the other materials.

| Metal Hydride | Density($g/cm^3$) |
|---|---|
| $\mathrm{Mg(BH_4)_2}$ | 1.48 |

*Table 3.3: Specification of Shield Material*

The main purpose of including the shield layer is to reduce nuclear heating and protect the conducting coils from nuclear as well as neutron-irradiation damage.

### 3.5.4 Stainless Steel 316

As it is necessary to achieve plasma confinement for a functioning fusion reactor device, a vacuum vessel is required in which the plasma can remain confined by the magnetic field induced by the conducting coils. The vacuum vessel is made out of stainless steel. The material used is Stainless Steel 316. This particular grade of stainless steel is a chromium nickel austenitic stainless steel containing molybdenum (Mo). The molybdenum addition enhances the corrosion resistance in halide environments as well as in reducing acids such as sulphuric and phosphoric acid. It resists atmospheric corrosion as well as in moderately oxidizing environments.

The specifications of the stainless steel used have been mentioned in table 3.4.

| **Properties of Stainless Steel** | **Value/Composition** |
|---|---|
| *Density* | 7.90 g/$cm^3$ |
| *Name of Element* | |
| Nitrogen | 0.1 wo |
| Silicon | 0.75 wo |
| Sulphur | 0.03 wo |
| Phosphorus | 0.45 wo |
| Manganese | 2 wo |
| Carbon | 0.08 wo |
| Chromium | 18.0 wo |
| Nickel | 14.0 wo |
| Molybdenum | 3.0 wo |
| Iron | 62.0 wo |

*Table 3.4: Specification of Stainless Steel 316 [15])*

### 3.5.5 Copper

The layer of copper(pure) depicts the conducting coils usually used in any fusion reactor devices. The conducting coils can also be replaced by some superconducting materials.

| Element | Composition(ao) | Density($g/cm^3$) |
|---|---|---|
| Copper(Cu) | 99.5 | 8.96 |

*Table 3.5: Specification of Copper*

## 3.6 D-T Model

The objective behind this model is already mentioned in section 3.3. In this model, the geometry consists of a thin layer(1 cm) of vanadium alloy V-4Cr-4Ti followed by the breeding layer of liquid lithium followed by the second layer(2 cm) of vanadium alloy. This replicates liquid lithium being sealed in vanadium alloy containers. Then the shield layer of metal hydride is then followed by the third layer (1 cm) of vanadium alloy. Then comes the structural stainless steel layers (4 cm) replicating the boundary of the vacuum vessel followed by copper layers (20 cm thick) depicting the conducting coils.The surfaces of theses layers are shared either on one side or on both sides. The second layer of vanadium alloy (2 cm thickness) replicates 1 cm thickness vanadium alloy container in which the liquid lithium is sealed and the other 1 cm replicates the vanadium-alloy container surface in which the shield material is contained followed by the third layer of vanadium alloy replicating the closing surface of container. The details about the dimensions as well as boundary conditions are already mentioned in section 3.3.

In this case, the fixed neutron source has an energy of 14.1 MeV.

The basic principle of this model lies in the below mentioned nuclear fusion reaction:

$\mathrm{D} + \mathrm{T} \longrightarrow {}^{4}_{2}\mathrm{He} + {}^{1}_{0}\mathrm{n}\,(14.1\,\mathrm{MeV})$

As discussed in Tritium Breeding Mechanism (section 2.1.1), this 14.1 MeV neutron then undergoes a neutron-induced reaction with natural liquid lithium (mixture of $^{6}Li$ and$^{7}Li$) to breed tritium. The purpose of the liquid lithium is not limited in Tritium production rather it serves as a self-cooling system as well as act as a shield too since it absorbs a portion energy of the highly energetic neutrons.

Initially the central cylinder of radius 110 cm as mentioned in section 3.3 was created and then each layer has been added one after another. The thickness of the liquid lithium layer was decided and fixed to 55 cm by calculating the cumulative TBR. Initially the liquid lithium layer was much thicker as compared to the present one. In the plot below it can be seen that with the vanadium and lithium layers , at 45 cm the TBR value is 1.02 (more than one). The thickness was increased from 45 cm to 55 cm after adding the later layers since the the TBR value became less than 1 due to deposition of neutron energy in shield material as well as in other structural materials.

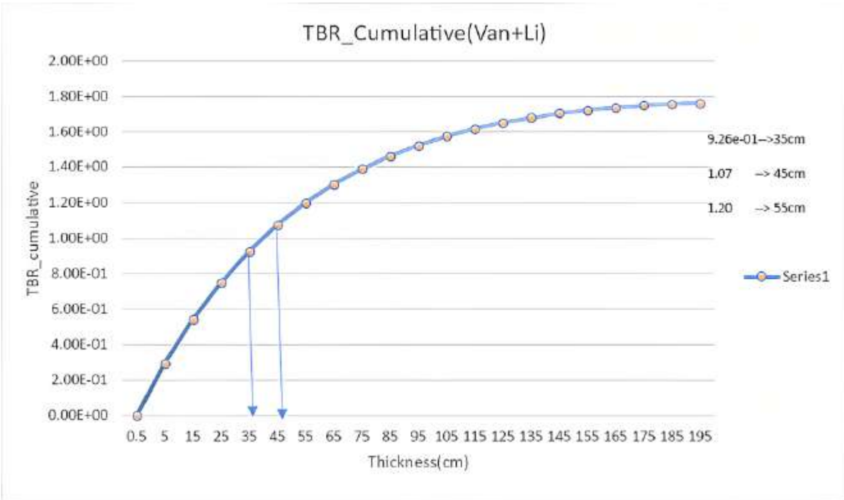


*Figure 3.4: Plot to obtain optimal TBR value*

The thickness of the shield material has been decided based on the amount of energy deposition in the conducting coils (copper layers). The objective behind is to achieve least amount of energy deposition but on the contrary the cost also needs to be taken into account. Initially a comparatively thicker (more than 40 cm )layer of shield(metal hydride) was added. Then the total amount of energy deposited (Total Energy Deposition), energy deposited in the copper layers(Total Energy Deposition in Cu) and the ratio $\frac{\text{Total Energy Deposition in Cu}}{\text{Total Energy Deposition}}$ was calculated. Based on consecutive simulations with different thickness of shield material and the Total Energy Deposition in Cu and the thickness of shield material has been concluded.

The thicknesses of all the layers included in D-T model are mentioned in the below table:

| Layer Name | Thickness(cm) |
|---|---|
| $V-4\,Cr-4\,Ti$ | 1 |
| Lithium | 55 |
| $V-4\,Cr-4\,Ti$ | 2 |
| $Mg(BH_4)_2$ | 40 |
| $V-4\,Cr-4\,Ti$ | 1 |
| Stainless Steel | 4 |
| Copper | 20 |

*Table 3.6: Geometry Specification of D-T Model*

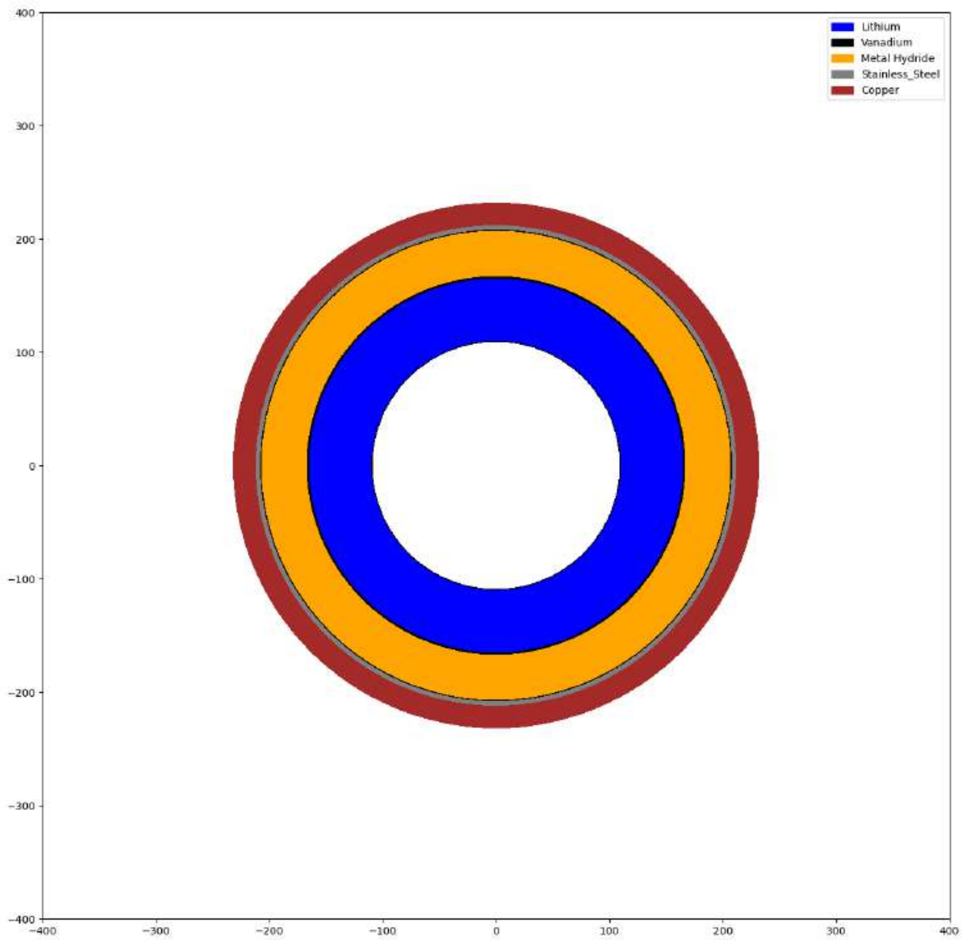


*Figure 3.5: Geometry of D-T Model*

## 3.7 D-D Model

The basic principle of this model lies in the below mentioned nuclear fusion reaction:

1. $\mathrm{D} + \mathrm{D} \longrightarrow \mathrm{T} + {}^{1}_{1}\mathrm{p}$
2. $\mathrm{D} + \mathrm{D} \longrightarrow {}^{3}_{2}\mathrm{He} + {}^{0}_{1}\mathrm{n}\,(2.45\,\mathrm{MeV})$

The basic difference between the above discussed D-T model and D-D model is that unlike the former model, there is no need of breeding in the latter one since tritium is produced in D-D reaction branch 1. Although, the purpose of this model is already mentioned in 3.3, it is beneficial to recapitulate that this model is built to check the thickness of shield required in order to moderate the neutrons produced as a result of D-D reaction and compare it with that required in case of D-T model.

It has been mentioned in section 1.2.2 that one of the branches of D-D reaction produces 2.45 MeV neutron alongwith $3He$ and another branch produces tritium and proton. There's a possibility that this product tritium can undergo an induced D-T reaction with one of the reactant deuterium and produce high energy 14.1 MeV neutrons. Hence, the following two scenarios has been considered in case of D-D model . In both of the below discussed models (case 1 and case 2), no lithium layer exists as there is no need to breed tritium.

### 3.7.1 Case 1

The geometry consists of a thin vanadium alloy(1 cm), followed by shield layer (55 cm) and then the second layer of vanadium alloy (1 cm). The idea of adding vanadium layers is same as in case of 3.6. They basically replicate the wall surfaces of the vanadium alloy containers in which the metal hydride is being sealed. Then the geometry is followed by the structural stainless steel layers and copper layers. The thickness of the vacuum vessel and the conducting coils are same and fixed for both the models. The fixed neutron source in this case has an energy of 14.1 MeV. The thickness of the shield layer has been decided based on the same concept mentioned in 3.6.

The thicknesses of all the layers included in this case of D-D model are mentioned in the below table:

| Layer Name | Thickness(cm) |
|---|---|
| $\mathrm{V{-}4\,Cr{-}4\,Ti}$ | 1 |
| $\mathrm{Mg(BH_4)_2}$ | 55 |
| $\mathrm{V{-}4\,Cr{-}4\,Ti}$ | 1 |
| Stainless Steel | 4 |
| Copper | 20 |

*Table 3.7: Geometry Specification of D-D Model for a 14.1 MeV neutron source*

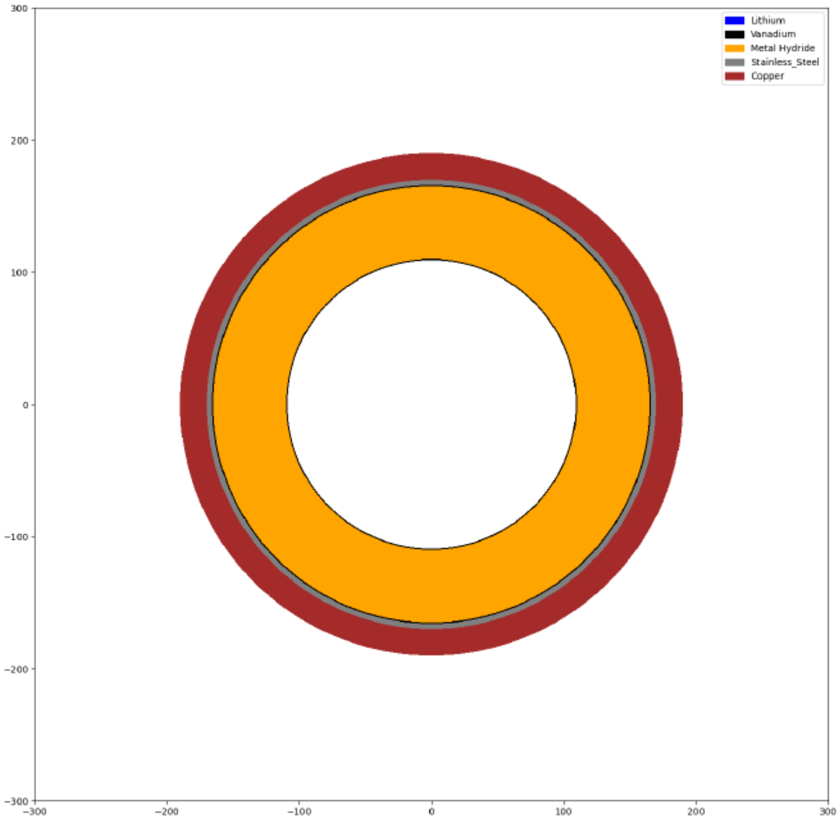


*Figure 3.6: Geometry of D-D Model (14.1 MeV)*

### 3.7.2 Case 2

In this case, the objective and geometry is similar to the one as mentioned in section 3.7.1 except the thickness of the shield and the fixed neutron source has an energy of 2.45 MeV. This model is based on D-D reaction branch 2. The idea of deciding the shield thickness is based on the same concept as mentioned in sections 3.6 and 3.7.1. It can be clearly observed from the table 3.8 that this case has the least thick shield layer amongst the all three scenarios which is quite logical considering the lower energy of source neutrons.

The thicknesses of all the layers included in this case of D-D model are mentioned in the below table:

| Layer Name | Thickness(cm) |
|---|---|
| $\mathrm{V{-}4\,Cr{-}4\,Ti}$ | 1 |
| $\mathrm{Mg(BH_4)_2}$ | 20 |
| $\mathrm{V{-}4\,Cr{-}4\,Ti}$ | 1 |
| Stainless Steel | 4 |
| Copper (Cu) | 20 |

*Table 3.8: Geometry Specification of D-D Model for a 2.45 MeV neutron source*

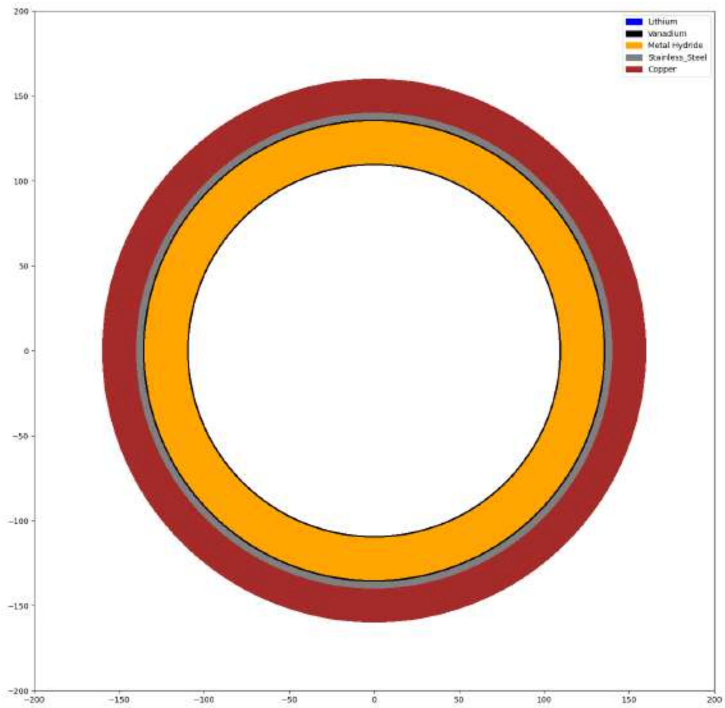


*Figure 3.7: Geometry of D-D Model (2.45 MeV)*

The aim behind developing these aforementioned models is to perform a one-dimensional radial analysis as the neutrons traverse through different layers by depositing energy. The parameters which have been studied as a part of this project are leakage fraction, TBR(to score the the amount of tritium breeding), Flux behaviour, Energy deposition. Besides, the alpha-particles production has also been looked at. The flux and energy deposition behaviour is studied to check whether the neutrons are well-moderated and shielded to avoid unnecessary heating of conducting coils since cooling coils to cryogenic temperatures is expensive. Also, high dosage of neutron-irradiation can cause severe structural damage to the materials. Besides, because of highly penetrating characteristic of neutron-irradiation, it is harmful for the technicians in aspects of their health, which needs to be taken into account.

All the models discussed in Chapter 3 have been created and simulated using the open-source neutron transport code, OpenMC.

# Chapter 4

# Introduction to OpenMC

This chapter is dedicated to introduce the open source Monte Carlo Neutron Transport, OpenMC to the readers and discuss the application of its functionalities and their usage in this project.

## 4.1 Why a Monte-Carlo based code? [16]

The physical processes involved for the evolution of a group of particles over time is determined by several probability distributions. For example, if we consider a particle moving through a substance, there exists a distribution that describes the probability of the distance it will travel before its next collision (can be called as an exponential distribution). Additionally, when the particle collides with a nucleus, there are probabilities associated with each possible reaction that can occur. Although the behavior of individual particles cannot be predicted, the collective behavior of a large population of particles originating from the same source follows well-defined patterns.

When the probability distributions governing the particle's movement are known, it is possible to simulate the process of individual particles streaming and colliding with nuclei using a computer technique called Monte Carlo simulation. By simulating a sufficient number of particles, the average behavior can be determined accurately, with minimal statistical error, as guaranteed by the central limit theorem. To be more precise, the central limit theorem states that the variance of the sample mean for estimating a physical parameter through Monte Carlo will decrease inversely proportional to the number of realizations(i.e the number of particles being simulated).

$$\sigma^2 \propto \frac{1}{N} \tag{4.1}$$

where $\sigma^2$ is the variance of the sample mean and N is the number of realizations.

Pros and Cons of Monte Carlo methods:

- Pro: No mesh generation is required to build geometry. By using constructive solid geometry, it's possible to build complex models with curved surfaces.
- Pro: Monte Carlo methods can be used with either continuous-energy or multi-group cross sections.

- Pro: Running simulations in parallel is conceptually very simple.
- Con: Because they rely on repeated random sampling, they are computationally very expensive.
- Con: A simulation doesn't automatically give you the global solution everywhere – you have to specifically ask for those quantities you want.
- Con: Even after the problem is converged, it is necessary to simulate many particles to reduce stochastic uncertainty.

## 4.2 About OpenMC

The open source Monte Carlo code specializing in neutron and photon transport simulations, OpenMC, is originally developed by the computational reactor physics group of MIT(Massachusetts Institute of Technology, Cambridge, Massachusetts). In present day, there are various universities and laboratories worldwide who contribute to its development. OpenMC has the capability to perform various calculations such as k-eigenvalue, fixed source, and subcritical multiplication using models created through constructive geometry or imported from CAD software. These calculations can be done for both continuous energy and multigroup transport scenarios.

OpenMC simulates neutral particles (presently neutrons and photons) moving stochastically through an arbitrarily defined model that represents an real-world experimental setup. The experiment could be as simple as a sphere of metal or as complicated as a full-scale nuclear reactor. This is what's known as Monte Carlo simulation. [16]

OpenMC includes a rich Python API that offers many usability improvements over dealing with raw XML input files. OpenMC software is built on the Python programming language and provides a Python API(Application Programming Interface) for programmatic pre and post-processing. For ease of installation, the simulations are primarily run on a Linux operating system such as Linux Mint, Ubuntu etc. OpenMC is licensed under the MIT/X open source license. This permissive license allows any user to copy, modify, redistribute, and even sell the software if they so wish.

In this project, due to lack of availability of a Linux-based computer, a subsystem linux WSL2 on a Windows-based computer has been used, within which Ubuntu 22.04.2 has been installed. Then it has been proceeded with installation of OpenMC using conda followed by downloading Visual Studio Code (VS code) editor (since the user is more familiar with it and it has Python as well as Jupyter Notebook extension) within the remote linux-based system.. Then via the terminal of VS code editor the OpenMC environment was activated. Within the OpenMC environment, the Python 3.11 extension was downloaded. Initially, a python script file with .py extension was ran via the VS code terminal, later on it has been decided to switch to Jupyter Notebook to resolve the errors with ease. From a personal point of view, it would be recommended to use OpenMC in a Linux-based computers if available as most of the users are either using Linux or a Mac, which makes it easier to find solutions to the problems that appears. A Windows-64 bit system with a processor i3-10th generation has been used to carry on this project but seems a more updated system is better to use since computer faced a lot of freezing since downloading OpenMC and it also became unresponsive at times. [16] [17]

To perform an OpenMC simulation, the materials constituting the model must be declared. It is possible to use different elements and isotopes to compose a single material, specifying their abundances, overall density, and the temperature at which their properties need to be evaluated. All the defined materials must be collected and exported to an XML file, which serves as input for the simulation.

The model can be defined using constructive geometry, where combinations of planes, spheres, cylinders, and other shapes define regions in space called cells to allocate different materials. The collection of cells within a root universe constitutes the model, which also needs to be exported to an XML file. OpenMC can directly plot the geometry. The next crucial step involves selecting a source for the simulation. In the case of fusion reactor simulations, a "fixed source" is typically used, requiring the user to provide a source for the model. Various source options are available, and users have the flexibility to generate custom sources. The key parameters to specify are the energy of the emitted particles, the angular dependence, and the spatial distribution. An XML file must be generated to define the source as well.

After setting the general parameters of the simulation, such as the number of particles per batch and the number of batches, the user needs to declare the run mode (e.g., "fixed source" or "k-eigenvalue") in this section, which also needs to be exported to an XML file. At this point, the simulation can be executed, but the results would be rudimentary since the data to be counted has not been defined. The user must set up a tally object, specifying which reactions or events need to be counted during the simulation, such as absorption, leakages, tritium production, and more. OpenMC provides scripting support for post-processing analysis, allowing for mathematical manipulation of tally results or the generation of graphical representations.

### 4.2.1 Flow of the OpenMC Simulation [16]

OpenMC carries out particle-by-particle Monte Carlo simulation, ensuring that only one particle is tracked at a time within a single program instance. Prior to tracking any particle, the problem needs to be initialized. The following steps are involved in the above mentioned procedure:

- The input files are read and data structures are constructed to store information related to the geometry, materials, tallies, and other relevant variables.
- The pseudorandom number generator (PRNG) is initialized. PRNG refers to an algorithm that uses mathematical formulas to produce sequences of random numbers.
- The problem-specific continuous-energy or multi-group cross section data indicated in the given scenario is read.
- For a fixed source problem like the one I have used in this project, source sites are sampled from the designated source according to the specified conditions. The source sites consist of coordinates, a direction, and an energy. Both multi-group as well as eigenvalue problems can be simulated using OpenMC.

After the problem initialization is done, the actual transport simulation is proceeded. The following steps mentioned below describes the how the life of a single particle is being proceeded:

1. The attributes of the particle are initialized based on a previously sampled source site.
2. Based on the position coordinates of the particle, the program determines in which cell is the particle currently located.
3. The program evaluates the energy-dependent cross sections for the material in which the particle is presently situated. It should be noted that this evaluation encompasses the total cross section, which is not pre-calculated.

4. Depending on the bounding surfaces of the cell, the program decides the distance to the closest boundary of the particle's cell.

5. The distance to the next collision is sampled. Assuming, the total cross section of the material be $\Sigma_t$, the following mathematical expression describes the relation between the distance to the collision and the cross section:

$$d = \frac{ln\xi}{\Sigma_t} \tag{4.2}$$

   where $\xi$ is a pseudorandom number sampled from a uniform distribution on (0,1]

6. If the distance to the nearest boundary is shorter than the distance to the next collision, the particle will move forward towards the boundary. Subsequently, the process will reiterate starting from step 2. Conversely, the particle will undergo a collision, if the distance to collision is closer than the distance to the nearest boundary.

### 4.2.2 A Sample OpenMC Script

In this section, the steps involved in creating a model in OpenMC environment has been discussed and the corresponding code snippets using Python API has also been show alongside.

#### 4.2.2.1 Geometry Specification [16]

The geometry of a model in OpenMC is defined using constructive solid geometry (CSG), also sometimes referred to as combinatorial geometry. CSG allows a user to create complex regions using Boolean operators (intersection, union, and complement) on simpler regions. In order to define a region that we can assign to a cell, we must first define surfaces which bound the region. A surface is a locus of zeros of a function of Cartesian coordinates x, y, z.

For example:

- A plane perpendicular to the x-axis: $x - x_0 = 0$.
- A cylinder parallel to the z-axis: $(x - x_0)^2 + (y - y_0)^2 - R^2 = 0$.
- A sphere: $(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 - R^2 = 0$.

Defining a surface alone is not sufficient to specify a volume – in order to define an actual volume, one must reference the half-space of a surface. A surface half-space is the region whose points satisfy a positive or negative inequality of the surface equation. Thus, we say that the negative half-space of the sphere, is defined as the collection of points satisfying $f(x, y, z) < 0$, which one can reason is the inside of the sphere. Conversely, the positive half-space of the sphere would correspond to all points outside of the sphere, satisfying $f(x, y, z) > 0$.

In the Python API, surfaces are created via subclasses of openmc.Surface.

Each surface is characterized by several parameters. As one example, the parameters for a sphere are the x,y,z coordinates of the center of the sphere and the radius of the sphere. All of these parameters can be set either as optional keyword arguments to the class constructor or via attributes. When a surface is created, by default particles that pass through the surface will consider it to be transmissive, i.e., they pass through the surface freely. If your model does not extend to infinity in all spatial dimensions, you may want to specify different behavior for particles passing through a surface.

To specify a vacuum boundary condition, simply change the Surface.boundary_type attribute to 'vacuum'. Reflective and periodic boundary conditions can be set with the strings 'reflective' and 'periodic'. Vacuum and reflective boundary conditions can be applied to any type of surface. Periodic boundary conditions can be applied to pairs of planar surfaces. If there are only two periodic surfaces, they will be matched automatically.

Once a material is created and a region of space is defined, a cell that assigns the material to the region needs to be defined. Cells are created using the openmc.Cell class.

In this section, a snippet of an OpenMC code using Python API to create a specific geometry has been shown. The following code also includes definition of the regions and cells of the surfaces (or shared surfaces) using logical operators.

```
#example surfaces
inner_sphere_surface = openmc.Sphere(r=480)
middle_sphere_surface = openmc.Sphere(r=500) # note the extra surface
outer_sphere_surface = openmc.Sphere(r=600)

# above (+) middle_sphere_surface and below (-) outer_sphere_surface
blanket_region = +middle_sphere_surface & -outer_sphere_surface
# above (+) inner_sphere_surface and below (-) middle_sphere_surface
firstwall_region = +inner_sphere_surface & -middle_sphere_surface

# now we have two cells
blanket_cell = openmc.Cell(region=blanket_region)
firstwall_cell = openmc.Cell(region=firstwall_region)

# there are now two cells in the list
universe = openmc.Universe(cells=[blanket_cell, firstwall_cell])

# shows the plots, which still look the same for all directions
color_assignment = {blanket_cell: 'blue', firstwall_cell: 'red'}
plt.show(universe.plot(width=(1200, 1200), basis='xz', colors=color_assignment))
plt.show(universe.plot(width=(1200, 1200), basis='xy', colors=color_assignment))
plt.show(universe.plot(width=(1200, 1200), basis='yz', colors=color_assignment))
```

In this above snippet, the regions are not filled with any material. The regions defined are void.

### 4.2.3 Specifying Material

Materials in OpenMC are defined as a set of nuclides/elements at specified densities and are created using the openmc.Material class. Once a material has been instantiated, nuclides can be added with Material.addnuclide() and elements can be added with Material.addelement(). The third argument to Material.addnuclide() can also be 'wo' for weight percent. The densities specified for each nuclide/element are relative and are re-normalized based on the total density of the material. The total density is set using the Material.setdensity() method. The density can be specified in gram per cubic centimeter ($g/cm^3$), atom per barn-cm ($atom/b-cm$), or kilogram per cubic meter ($kg/m^3$).

Here's an example of the material definition in an OpenMC model using Python API has been described.

```
water_mat = openmc.Material()

# add each isotope with their relative abundance to material object
# note that H20 requires hydrogen to be multiplied by 2
water_mat.add_nuclide('H1', 2.*0.999885, percent_type='ao')
water_mat.add_nuclide('H2', 2.*0.000115, percent_type='ao')
water_mat.add_nuclide('O16', 0.99757, percent_type='ao')
water_mat.add_nuclide('O17', 0.00038, percent_type='ao')
water_mat.add_nuclide('O18', 0.00205, percent_type='ao')

# set material density
water_mat.set_density('g/cm3', 0.99821)
```

It is also required to define materials before defining the geometry as assigning materials to cells is also necessary when we want to use the geometry for particle transport.

Here's an example of the geometry with materials other than void:

```
#Defining lithium as a material
lithium_mat = openmc.Material(name='lithium')
lithium_mat.set_density('g/cm3', 2)
lithium_mat.add_element('Li', 1.0)

#Defining Tungsten as a material
tungsten_mat = openmc.Material(name='tungsten')
tungsten_mat.set_density('g/cm3', 19)
tungsten_mat.add_element('W', 1.0)

#Adding material To Blanket
blanket_cell = openmc.Cell(region=blanket_region)
blanket_cell.fill = lithium_mat  # this assigns a material to a cell

#Adding material To First Wall
firstwall_cell = openmc.Cell(region=firstwall_region)
firstwall_cell.fill = tungsten_mat  # this assigns a material to a cell
```

### 4.2.4 Defining Execution Setting Parameters

The next step is to specify execution settings through the openmc.Settings class and how many particles to run. In this section, a snippet of the code on how to define settings such as run mode, run strategy has been shown.

```
# Instantiate a Settings object
settings = openmc.Settings()
settings.particles = 10000 //No. of Source Particles
settings.batches = 20 //No. of batches the total no. of particles are divided in
settings.particle = "neutron" //type of source particle
```

//Runs a fixed-source calculation with a specified external source, specified in the Settings.source attribute.

```
settings.run_mode = 'fixed source'
```

### 4.2.5 Source Distribution

In this section, a snippet of the code creating and specifying source distribution has been shown.

```
    # initialises a new source object
my_source = openmc.Source()

# sets the location of the source to x=0 y=0 z=0
my_source.space = openmc.stats.Point((0, 0, 0))

# sets the direction to isotropic
my_source.angle = openmc.stats.Isotropic()

# sets the energy distribution to 100% 14MeV neutrons
my_source.energy = openmc.stats.Discrete([14e6], [1])
```

### 4.2.6 Final Step

Last but not the least, now the parameters needed to be studied for a particular model needs to be scored.

For example, the 'Flux' parameter is scored as follows:

//adding a cell filter so that the parameter is scored only in that particular cell

```
cell_filter = openmc.CellFilter(breeder_blanket_cell)
```

```
# added a cell tally for Flux
flux_tally = openmc.Tally(name='Flux')
flux_tally.filters = [cell_filter]
flux_tally.scores = ['flux']
tallies = openmc.Tallies([flux_tally])
```

Then the model can be run using the following code:

```
# Run OpenMC!
```

//geometry, materials, settings and tallies need to be exported as .xml files.

```
model = openmc.model.Model(geometry, materials, settings, tallies)
!rm summary.h5
!rm statepoint.*.h5
sp$_$filename = model.run()
```

The next steps involve, loading the output file and extracting simulation results as below. Here's a sample snippet:

```
# open the results file
sp = openmc.StatePoint(sp_filename)

# access the tally using pandas dataframes
```

```
flux_tally = sp.get_tally(name='TBR')
df_flux = flux_tally.get_pandas_dataframe() //returns the contents of the dataframe
```

The output values can be accessed using dataframe. Here's a sample snippet:

```
# sums up all the values in the mean column
flux_tally_result = df_flux['mean'].sum()

# sums up all the values in the std. dev. column
flux_tally_std_dev = df_flux['std. dev.'].sum()

# printing the results
print('Mean_Flux = ',flux_tally_result)
print('Standard deviation on the Flux tally is =', flux_tally_std_dev)
```

# Chapter 5

# Results and Analysis

This chapter is dedicated to discuss the various parameters studied for both the previously discussed fusion device models discussed in sections 3.6 and 3.7 followed by analysis and comparison.

Before discussing the results and the corresponding plots, it is necessary to discuss about the source settings, geometry and the different parameters associated to the source which are responsible for the following results.

| Source Parameters | Specifications |
|---|---|
| Source Particle | Neutron |
| Source Type | Fixed |
| Source Energy | 14.1 MeV/2.45 MeV |
| Number of Source Particle | 10000 |
| Number of batches | 20 |

*Table 5.1: Specifications of the Source*

The various parameters which have been scored to study and analyse the models include Tritium Breeding Ratio(TBR), Energy, Flux, Alpha particle production etc.

Besides,the number of particles which have crossed the vacuum boundary per source neutron has also been discussed, which is termed as Leakage Fraction. Leakage fraction is simply the fraction of the total number of particles that were eliminated by vacuum boundaries.

# 5.1 D-T model

In this section, the results obtained in case of D-T model as mentioned in 3.6 has been discussed.

## 5.1.1 Leakage Fraction

The leakage fraction for the D-T model is 0.00016.

## 5.1.2 Tritium Breeding Ratio

In OpenMC, TBR (tritium breeding ratio) is scored by scoring the (n,t) or (n, Xt) reaction rate. Here, X is a wildcard character, which catches any tritium production. This allows the tally to be recorded per nuclide so we can see which nuclide contributes to tritium production more.

The total value of TBR in case of D-T model for a 14.1 MeV neutron source is 1.15, the maximum value and minimum value being 1.53e-01 and 0.0e+00 respectively. In figure 5.1, it can be seen that the TBR is zero in the first layer of vanadium alloy. TBR starts from the beginning of the Liquid Lithium Layer and then gradually decreases until the end of the lithium layer and then there is a sudden free-fall at the middle of the second vanadium alloy layer followed by a slight increase at the beginning of the shield and then gradually decreases until zero.

A total amount of 1.15 TBR has been achieved. This value of TBR (TBR $\geq$ 1.1, self-sufficiency criterion achieved) has been achieved without enriching lithium-6. It has been obtained from the simulation that both lithium-6 and lithium-7 have contributed approximately 0.574 each (i.e 0.574*2 $=$ 1.148 $\approx$ 1.15). This implies that $^{6}Li$ and $^{7}Li$ have equally contributed in achieving the aforementioned TBR.

The variation of TBR in D-T model has been plotted in figure 5.1.

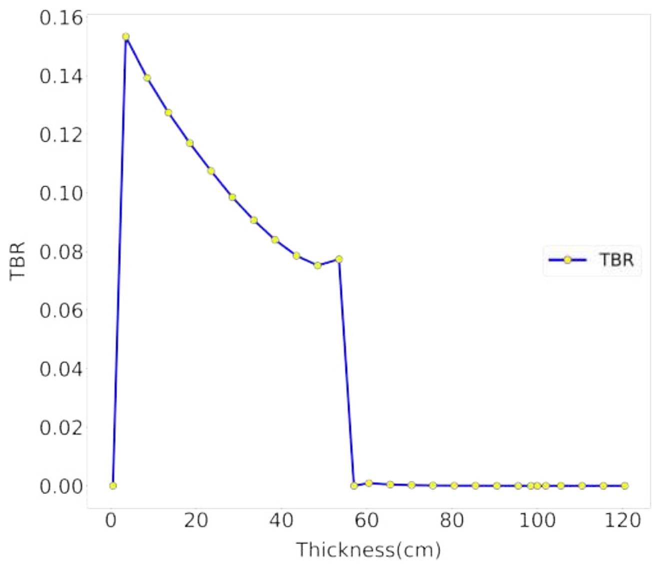


*Figure 5.1: Variation of TBR for D-T Model.*

The figure 5.2 shows the plot of the TBR data discussed in 5.1.2 in log scale.

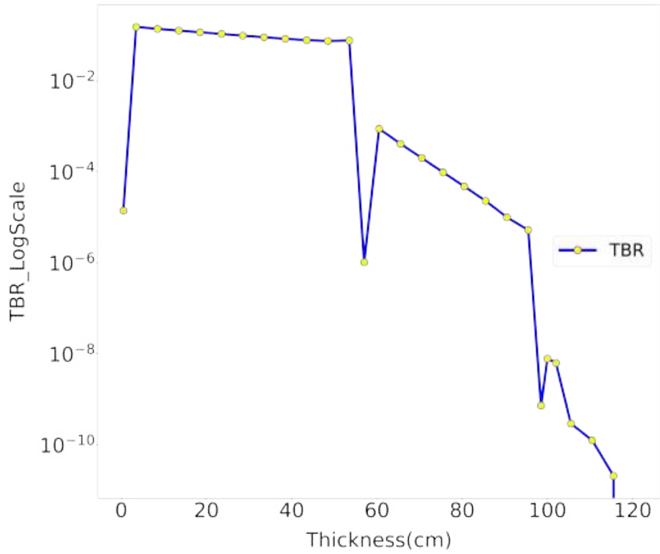


*Figure 5.2: Plot of TBR for D-T Model(Log Scale).*

### 5.1.3 Energy

The scored values of energy are in the units of eV/source-particle i.e. eV/source-neutron in this case. Whereas the plotted values in figure 5.3 are energy deposition fraction for each layer. The energy deposition fraction is a ratio between the (Total Quantity of Energy Deposited - Cumulative Quantity of Energy Deposited in each layer) and the Total Quantity of Energy Deposited and it has been calculated for each layer. The reason behind subtracting the cumulative energy deposition from the total energy is to get the energy deposition of each layer distinctively. Since the quantity on the y-axis is a fraction, it has no units. The same values have been re-plotted on log scale, shown in figure 5.4.

It is clearly visible that the deposition fraction is gradually decreasing. Maximum amount of energy has been deposited in the lithium layer which implies that the neutron energy has been utilised for tritium breeding followed by the shield layer. The descending trend of the energy deposition plot in the shield layer implies that the $Mg(BH_4)_2$ layer is fulfilling the purpose of shielding neutrons.

The total amount of energy deposition in the D-T model is 13.7 MeV/source-neutron, whereas the energy deposition in the copper layers (conducting coils) is $3.19 \times 10^2$ eV/source-neutron. This meets the criteria for protecting the coils from overheating and keeping them at cryogenic temperatures to maintain their superconductivity properties.

The variation in energy deposition fraction in different layers of D-T model has been shown in figure 5.3.

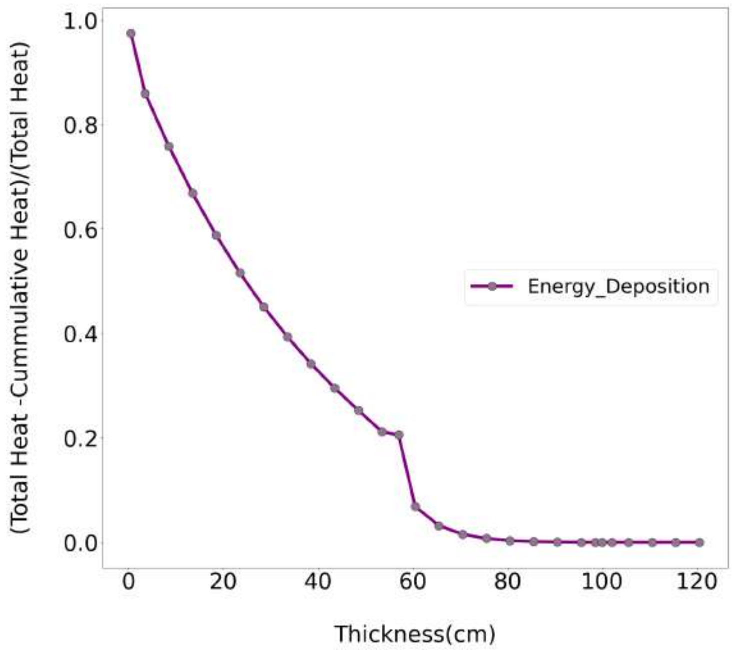


*Figure 5.3: Variation of Energy Deposition Fraction in various layers for the D-T Model.*

The plotted values of energy deposition fraction in figure 5.3 have been re-plotted in figure 5.4 on a log scale in the y-axis.

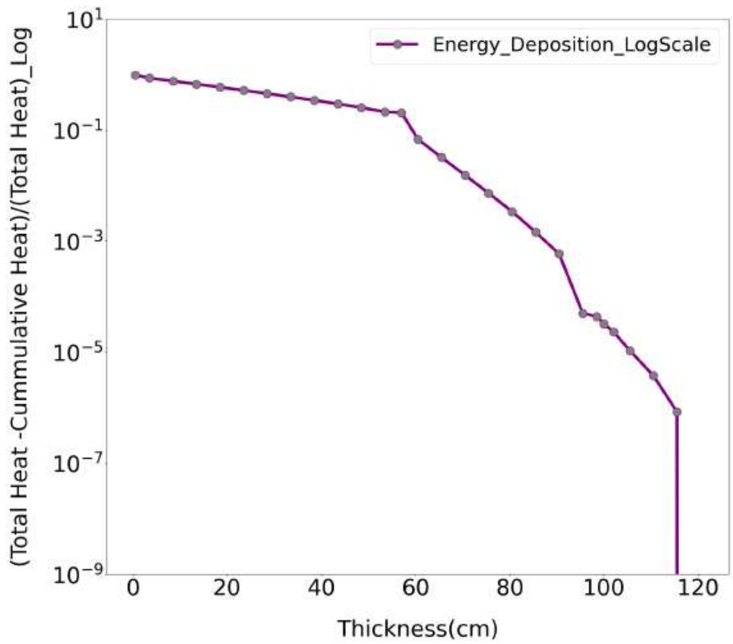


*Figure 5.4: Variation of Energy Deposition Fraction in various layers for the D-T Model (Log Scale).*

The table 5.2 contains the total amount of energy deposition, energy deposition in the copper layers and the fraction of energy deposition in copper layers and total energy deposition in D-T table:

| Quantity(Total) | Amount of Energy Deposited |
|---|---|
| Energy Deposited | 13.7 MeV/source-neutron |
| Energy Deposited in Cu Layers | 3.19e+02 eV/source-neutron |
| (Energy Deposited in Cu Layers)/(Energy Deposited) | 2.32e-05 |

*Table 5.2: Energy Depositions in case of D-T Model*

### 5.1.4 Flux

In OpenMC, the scored values of the parameter flux are in the units of particle*cm per source-particle i.e neutron*cm/source-neutron. The values obtained are basically weighted track length average or something akin to it (information has been gathered from the OpenMC discussion group). To simplify the dimension of the unit, the scored values have been divided by the volume of each layer and then multiplied by the corresponding area of that layer, which results flux values in the units of particles/source-particle i.e. neutrons/source-neutron.

The values of flux plotted in 5.5 are also in the units of neutrons/source-neutron. The plot in 5.5is descending in behaviour which is well-aligned with the fundamental concept as well as the desired flux behaviour.

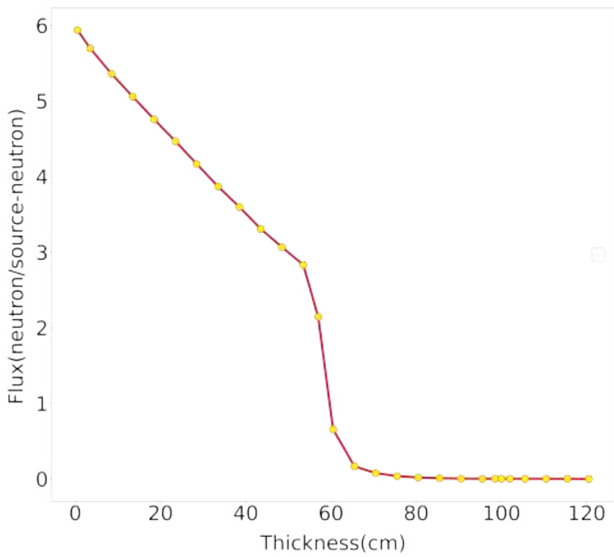


*Figure 5.5: Flux variation in the various layers for the D-T Model.*

The plot shown in figure 5.6 is of the same flux data as plotted in figure 5.5 with a log scale on the y-axis.

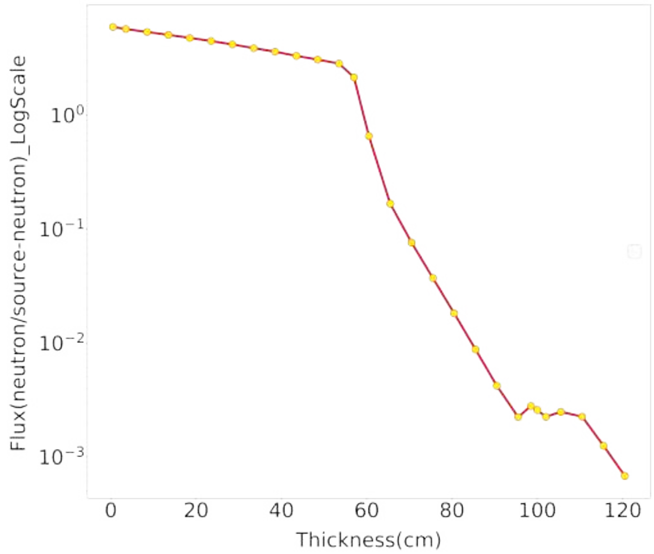


*Figure 5.6: Flux variation in the various layers for the D-T Model (Log Scale).*

### 5.1.5 Alpha Production

Here, alpha production refers to the production of Helium ($^4_2He$) as a result of neutron-induced reaction with the breeding as well as the structural materials. As per simulation a total of 1.8 alpha particles ( $^4_2He$) produced in this D-T model per source-neutron. Out of this total alpha particle production, $^6Li$ and $^7Li$ contributed 0.676 and 0.596 alpha-particles/source-neutron respectively.

## 5.2 D-D Model

In this section, the results for both cases of D-D model as mentioned in section 3.7 has been discussed.

### 5.2.1 Case1

The results for the first case of D-D model as mentioned in section 3.7.1, in which the energy of the neutron source was 14.1MeV has been discussed below:

#### 5.2.1.1 Leakage Fraction

The amount of leakage fraction is 0.00021.

#### 5.2.1.2 Energy

As discussed in section 5.1.3, the plotted values in figure 5.7 are energy deposition fractions which are ratios between (Total Quantity of Energy Deposited - Cumulative Quantity of Energy Deposited in each layer) and the Total Quantity of Energy Deposited and has no units but the values mentioned in table 5.3 are scored values and are in the units of eV/source.

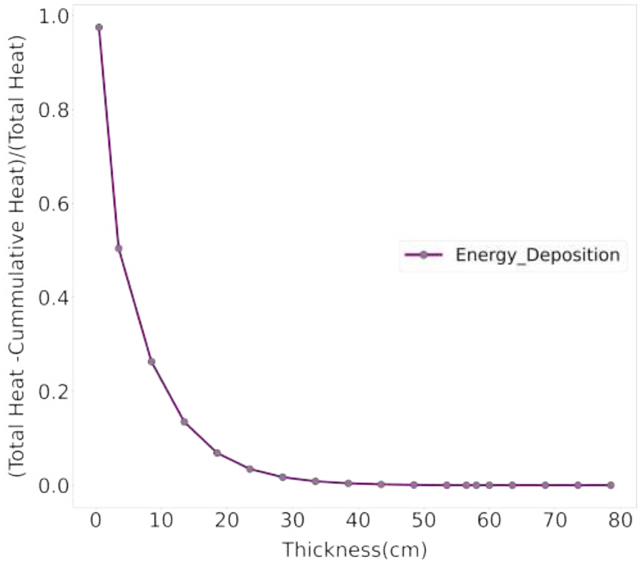


*Figure 5.7: Variation of Energy Deposition Fraction for a 14.1 MeV neutron source in D-D Model.*

The above plot clearly shows that the fraction of energy depositing in each layer is gradually decreasing as the source neutrons traverse through along the different layers of this model. The maximum deposition has occurred in the $Mg(BH_4)_2$ layer implying that the neutrons are properly shielded and are being prevented from transmitting heat to the conducting coils and hence preventing overheating, which is desirable to maintain superconductivity of the coils. The plotted values of deposition fraction in figure 5.7 have been re-plotted in figure 5.8 with a log scale in y-axis.

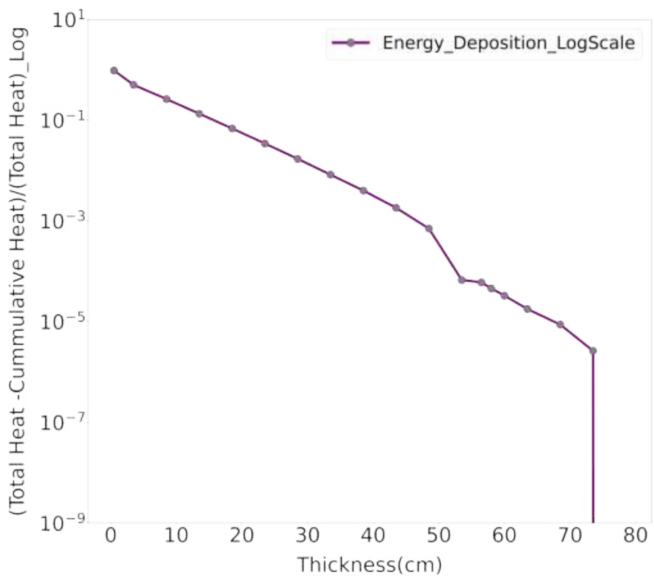


*Figure 5.8: Variation of Energy Deposition Fraction in case of D-D Model for a 14.1 MeV neutron source (LogScale).*

The table 5.3 contains the total amount of energy deposition, energy deposition in the copper layers and the fraction of energy deposition in copper layers and total energy deposition in case of the model as discussed in section 5.2.1:

| Quantity(Total) | Amount of Energy Deposited |
|---|---|
| Energy Deposited | 1.26e+07 eV/source |
| Energy Deposited in Cu Layers | 4.14e+02 eV/source |
| (Energy Deposited in Cu Layers)/(Energy Deposited) | 3.289e-05 |

*Table 5.3: Variation of Energy Depositions in case of D-D Model for a 14.1 MeV neutron source.*

#### 5.2.1.3 Flux

The plotted values of flux in 5.9 are in the units of neutron/source-neutron and the reason behind is same as that has been mentioned in section 5.1.4.

The plot is descending in behaviour.

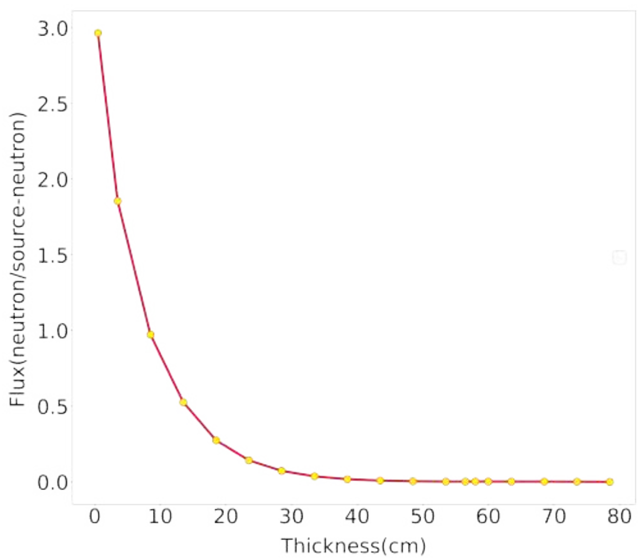


*Figure 5.9: Variation of Flux for a 14.1 MeV neutron source in D-D Model.*

The same flux data plotted in figure 5.9 has been re-plotted with a log scale on y-axis in figure 5.10.

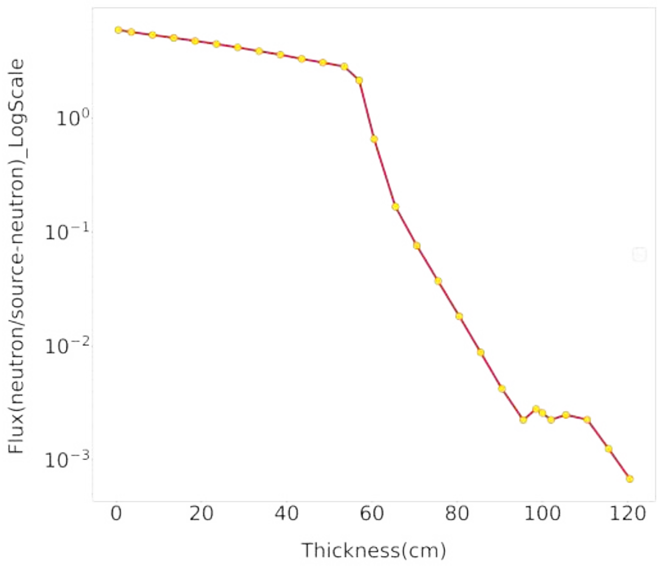


*Figure 5.10: Variation of Flux for a 14.1 MeV neutron source in D-D Model (LogScale).*

### 5.2.2 Case2

The results for the second case of D-D model, in which the energy of the neutron source was 2.5 MeV as mentioned in section 3.7.2 has been discussed below.

#### 5.2.2.1 Leakage Fraction

The Leakage Fraction is 0.00011.

#### 5.2.2.2 Energy

As discussed in section 5.1.3 and 5.2.1.2, the plotted values in figure 5.11 are energy deposition fraction [ratio between ( Total Quantity of Energy Deposited - Cumulative Quantity of Energy Deposited in each layer) and the Total Quantity of Energy Deposited] and has no units. But the values mentioned in table 5.4 are the scored values itself and are in the units of eV/source-neutron.

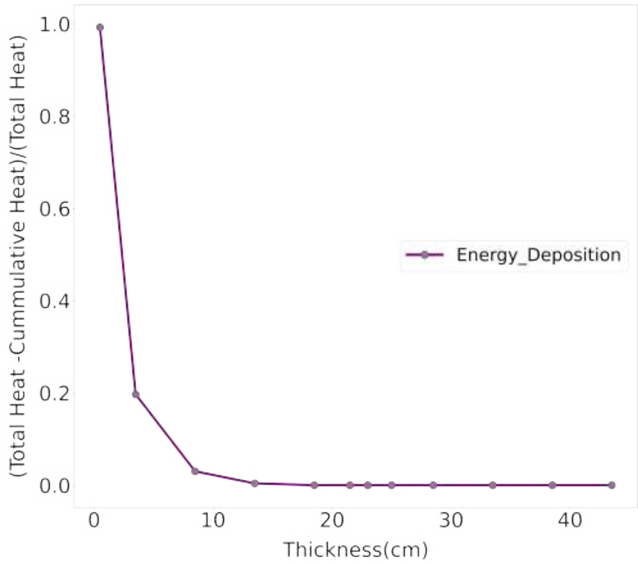


*Figure 5.11: Variation of Energy Deposition Fraction for a 2.45 MeV neutron source in D-D Model.*

The plotted values of energy deposition fraction in figure 5.11 have been re-plotted in figure 5.12 on a log scale in y-axis.

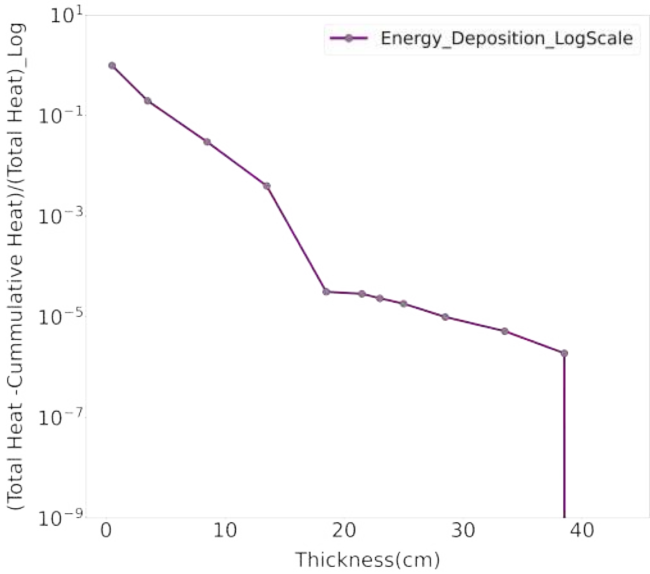


*Figure 5.12: Variation of Energy Deposition Fraction for a 2.45 MeV neutron source in D-D Model(Log Scale).*

The table 5.4 contains the total amount of energy deposition, energy deposition in the copper layers and the fraction of energy deposition in copper layers and total energy deposition in case of the model as discussed in section 3.7.2:

| Quantity(Total) | Amount of Energy Deposited |
|---|---|
| Energy Deposited | 4.60e+06 eV/source-neutron |
| Energy Deposited in Cu Layers | 8.43e+01 eV/source-neutron |
| (Energy Deposited in Cu Layers)/(Energy Deposited) | 1.83e-05 |

*Table 5.4: Energy Depositions in case of D-D Model for a 2.45 MeV neutron source*

#### 5.2.2.3 Flux

As mentioned in sections 5.1.4 and 5.2.1.3, the plotted values of flux in figure 5.13 are also in the units of neutron/source-neutron.

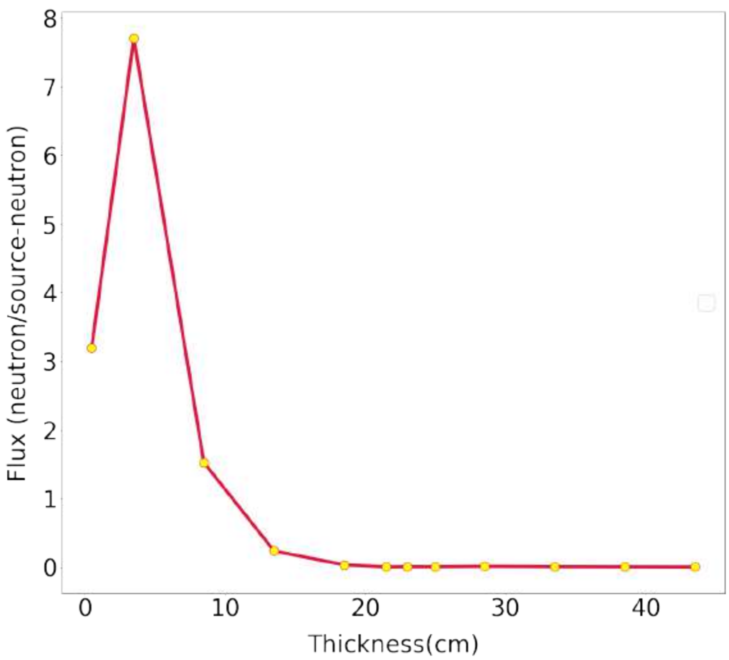


*Figure 5.13: Variation of Flux for a 2.45 MeV neutron source in D-D Model.*

Similar to figure 5.9, plot in figure 5.13 is also descending in behaviour.

The same flux data plotted in figure 5.13 has been re-plotted with a log scale on y-axis in figure 5.14.

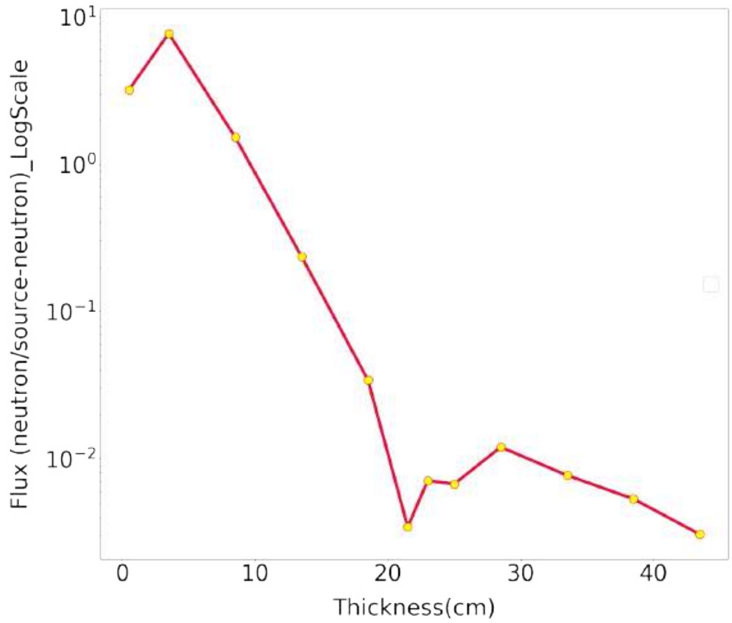


*Figure 5.14: Variation of Flux for a 2.45 MeV neutron source in D-D Model(Log Scale).*

## 5.3 Discussions

It has been clearly observed that achieved TBR has successfully fulfilled self-sufficiency criterion in case of D-T model with the provided breeding blanket layer of 55 cm thickness. Also, the provided thickness(40 cm) of the shield layer of the D-T model has turned out to fulfill the desirable requirement of shielding neutrons and minimum energy deposition in copper coils enhancing to maintain the superconductive property of the conducting coils. The required thickness of the shield layer in case of D-T model is comparatively lesser than that the thickness (55 cm) of the shield layer of D-D model (Case 1) since the breeding blanket also serves as an additional shielding in the former model whereas it's not the case for the latter model provided the neutron energy (14.1 MeV) is same for both the scenarios.

The required shield layer thickness of D-D Model (case 2) is relatively very less amongst the three scenarios discussed, because the energy of the source neutron is very low (2.45 MeV) as compared to case 1 of D-D model as well as D-T model .

Besides, simultaneously it is also desired to achieve the least leakage fraction. Amongst the three discussed cases, D-D model with a 2.45MeV neutron source has the least leakage fraction of 0.00021, which is obvious because of slow neutrons whereas D-D with 14.1 MeV source neutron has 0.00021 and D-T model has 0.00016 leakage fraction respectively.

The fraction of energy deposited in copper coils in case of D-T model has been used as reference to decide the thickness of shield in both cases of D-D model so that the same order of magnitude is maintained and the purpose protecting the coils from excess overheating is fulfilled. The thickness of the structural stainless steel and coils( copper layer) has been kept fixed for both of the models. The advantage of D-D model over D-T model is that there is no need of tritium breeding as Tritium is produced as a product from one of the branches of D-D fusion reaction. But the reaction cross-section of D-D reaction is very low as compared to that of D-T reaction. Hence, it can be concluded that D-T model is more feasible.

# Chapter 6

# Conclusions and Future Work

It is now clearly evident from the above discussions in Chapter 5 and section 5.3 that D-T model is much more efficient than the both of the scenarios of D-D model as it fulfills the TBR criterion, which is the primary one to be considered. Alongside the leakage fraction is also low. Considering, the Breeding Ratio as well as reaction cross section, it is justified that D-T model is the best suitable one.

TBR represents the ratio of tritium produced to tritium consumed in a fusion reactor. A TBR of 1.0 means the reactor breaks even (produces as much tritium as it consumes). Achieving a TBR $\geq 1.1$ is crucial for self-sufficiency. The 10% margin (the additional 0.1 in the TBR) accounts for uncertainties in various factors such as neutron transport calculations, material properties, tritium extraction efficiencies. During reactor operation, some tritium may be lost due to leakage, inefficiencies in breeding, or during extraction and handling. The margin helps to compensate for these losses. During maintenance, tritium production may be reduced or halted. A higher TBR ensures a sufficient tritium reserve to cover these periods without disrupting reactor operation. Producing tritium in-situ (via breeding) is more cost-effective than purchasing it from external sources.

If a reactor's TBR is exactly equal to 1.0, even small inefficiencies or losses could lead to a tritium deficit, jeopardizing reactor operation. A TBR of 1.1 means that for every 10 grams of tritium consumed, 11 grams are produced. In this study, 11.5 grams (TBR = 1.15) are produced per 10 grams of tritium consumption, with a margin of 15% to account for potential losses and uncertainties. Also, blanket doesn't cover the entire area around plasma.

On the contrary it is also desirable to avoid exceeding TBR beyond requirement because:

- Handling of radioactive Tritium can be challenging
- Higher TBR often means more neutron interactions, which can lead to increased radiation damage to reactor materials. This can affect the longevity and reliability of structural components.
- Neutron interactions with lithium and other materials can produce helium, which can cause swelling and embrittlement of structural materials.
- Increased tritium breeding can result in higher heat loads within the blanket. Efficient thermal management systems are required to handle this heat without compromising reactor performance.

In order to improve TBR atomic number density of $^6$Li is increased in the lithium due its low abundance in the natural form. Hence, consequent studies will include enriched $^6Li$

As it is well known that the blanket region is far from the plasma and $^6$Li has higher reaction cross-section for thermal neutrons resulting into efficient tritium breeding. Whereas, the reaction $7Li(n, n'T)\alpha$ the threshold that reacts from 2.5MeV, hence neutron capture is possible only when the neutrons are not much decelerated which is not the reality.

In future, simulations can be done using other liquid breeding blanket material,shield material. The structural materials can also be varied and compared. Also, in the existing models, it is planned to study the displacement per atoms for specific materials used.

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