Evaluation of the effects of ionizing radiation in ITER’s Plasma Position Reflectometry System

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Thesis for the degree of Master in

Mechanical Engineering

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October 2016
TO MY FAMILY
ACKNOWLEDGEMENTS

I would like to extremely thank to all the people whose names might not be enumerated and organisms that have contributed and made possible for me to do this exciting undertaking.

First of all, I express my deeply gratitude to my supervisors. Without them I could have not achieved a good level of motivation and learning on the topic. I could not be more satisfied with Hugo Policarpo and Raul Luis for their guidance, patience, kindness, endless encouragement and attention.

I would also like to thank my colleagues in the Instituto de Plasmas e Fusão Nuclear (IPFN), who have aided me in the understanding of the programs used, and the International Offices of the IST and ETSII for giving me the chance to do this passionate master thesis abroad and be able to grow personally. Moreover, I would like to specially thank to Professor Miguel Tavares da Silva for giving me the chance of doing the master thesis in the area I was looking for. I appreciate he put me into contact with my supervisors from the IST.

Finally, my family and friends have been decisive in the making of the project. They have given me all kind of unconditional support for which I will be eternally grateful.
No ITER (International Thermonuclear Experimental Reactor), o sistema de Reflectometria de Posição de Plasma (PPR) estará exposto a elevados níveis de radiação ionizante: neutrons provenientes das reações de fusão nuclear e fotões gerados nas interações nucleares com os materiais circundantes. O principal objectivo desta Tese é contribuir para o estudo do efeito das cargas nucleares nos componentes do sistema PPR através de cálculos de deposição de energia, complementando cálculos de distribuição de temperaturas efectuados em trabalhos anteriores com cálculos de DPA (Displacement per Atom), um parâmetro importante para avaliar os danos provocados nos materiais pela exposição à radiação. O programa de simulação por métodos de Monte Carlo MCNP6 e o software de Análise dos Elementos Finitos ANSYS foram usados nas análises neutónica e térmica, respectivamente, juntamente com o programa de processamento de secções eficazes NJOY.

O valor máximo de deposição de energia verifica-se nas extremidades das antenas, directamente expostas ao plasma. A temperatura máxima atingida nas antenas juntamente com os valores de DPA calculados mostram que é necessário optimizar o sistema para cumprir os requisitos do ITER. Adicionalmente, desenvolveu-se uma interface MATLAB-MCNP-ANSYS, que permite automatizar análises térmicas envolvendo cálculos de neutónica para um sistema de blindagem.

**Palavras-Chave:** Fusão nuclear, sistema de Reflectometria de Posição de Plasma, Monte Carlo, MCNP6, Elementos Finitos, ANSYS, Análise Termo-Mecânica.
ABSTRACT

In the International Thermonuclear Experimental Reactor (ITER), the Plasma Position Reflectometry (PPR) system will be exposed to high levels of ionizing radiation: neutrons from the nuclear fusion reaction and prompt photons from the nuclear interactions with the surrounding materials. The aim of this Thesis is to contribute to the study of the effect of the nuclear loads in the PPR components by estimating the power density in each cell of the PPR and complementing the results of temperature distribution from a previous work by calculating the Displacement Per Atom (DPA) in each component, an important parameter that estimates the radiation damage in the materials.

The maximum power density is reached at the tips of the antennas, as they are directly exposed to the plasma. The maximum temperature achieved in the antennas together with the calculated DPAs show that optimization of the PPR system is needed in order to comply with ITER's requirements. Furthermore, an interface MATLAB-MCNP-ANSYS was developed that permits to automatize the procedure for a coupled neutronics and thermal analysis of a layered shielding sphere.

KEY WORDS: NUCLEAR FUSION, PLASMA POSITION REFLECTOMETRY SYSTEM, MONTE CARLO, MCNP6, FINITE ELEMENTS, ANSYS, THERMO-MECHANICAL ANALYSIS.
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<td>ANSYS</td>
<td>Commercial code of Finite Elements by ANSYS, INC.</td>
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<tr>
<td>ASCII</td>
<td>American Standard Code for Information Interchange</td>
</tr>
<tr>
<td>BM</td>
<td>Blanket Modules</td>
</tr>
<tr>
<td>CAD</td>
<td>Computer Aided Design</td>
</tr>
<tr>
<td>CC</td>
<td>Correction Coils</td>
</tr>
<tr>
<td>CS</td>
<td>Central Solenoid</td>
</tr>
<tr>
<td>DD</td>
<td>Deuterium-Deuterium</td>
</tr>
<tr>
<td>DT</td>
<td>Deuterium-Tritium</td>
</tr>
<tr>
<td>ELM</td>
<td>Edge-Localized Mode</td>
</tr>
<tr>
<td>ENDF</td>
<td>Evaluated Nuclear Data File</td>
</tr>
<tr>
<td>ENOVIA</td>
<td>Product Lifecycle Management tool (Dassault Systèmes)</td>
</tr>
<tr>
<td>F4E</td>
<td>Fusion For Energy, European Union's Joint Undertaking for ITER and the Development of Fusion Energy</td>
</tr>
<tr>
<td>FE</td>
<td>Finite Element</td>
</tr>
<tr>
<td>FENDL</td>
<td>Fusion Evaluated Nuclear Data Library</td>
</tr>
<tr>
<td>ITER</td>
<td>International Thermonuclear Experimental Reactor</td>
</tr>
<tr>
<td>JANIS</td>
<td>Java-based Nuclear Data Information System</td>
</tr>
<tr>
<td>JEFF</td>
<td>Joint Evaluated Fission and Fusion File</td>
</tr>
<tr>
<td>JET</td>
<td>Joint European Torus</td>
</tr>
<tr>
<td>MATLAB</td>
<td>Commercial code for calculus MATrix LABoratory</td>
</tr>
<tr>
<td>MCAM</td>
<td>Monte Carlo Modelling Interface Program</td>
</tr>
<tr>
<td>MCNP</td>
<td>Monte Carlo N-Particle code</td>
</tr>
<tr>
<td>PENDF</td>
<td>Pointwise Evaluated Nuclear Data File</td>
</tr>
<tr>
<td>PF</td>
<td>Poloidal Field</td>
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<tr>
<td>PPR</td>
<td>Plasma Position Reflectometry</td>
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<tr>
<td>SolidWorks</td>
<td>CAD software developed by Dassault Systèmes</td>
</tr>
<tr>
<td>SpaceClaim</td>
<td>CAD software developed by SpaceClaim Corporation</td>
</tr>
<tr>
<td>STEP</td>
<td>Standard for the Exchange of Product model data</td>
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<tr>
<td>TF</td>
<td>Toroidal Field</td>
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<td>VS</td>
<td>Vertical Stability</td>
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1 INTRODUCTION

1.1 Context

Energy is vital for life. It is needed for food, heat and other key factors like electricity and mobility in order to guarantee a good standard of living. Since 2012, the world’s electricity demand is increasing at an average rate of 1.9%, whereby 80% of the energy’s consumption is based on fossil fuel [1][2]. The primary natural resources used to produce energy are: fossil fuels (coal, oil and natural gas), nuclear fuels (from fission and fusion) and sunlight, which is the driver for most renewables.

Currently, the energy demand is increasing, making CO₂ emissions a major concern. The global average concentration of CO₂ in the Earth’s atmosphere is increasing: from 396.85 parts per million (ppm) in August 2015 to 400.47 ppm in August 2016 [3]. It warms the planet and excess carbon in the ocean makes the water more acidic, constituting a danger to the environment and habitat. Thus, new energy production will face the constraint of reducing the greenhouse gas emissions. As all fossil fuels produce greenhouse gases, the increasing energy demand will have to be met by a combination of nuclear, hydroelectric and other renewable (e.g. wind, solar, geothermal) sources. Production of synthetic fuels, ethanol or hydrogen may be used to replace gasoline and diesel fuel. Apart from CO₂ production, each of the existing energy options faces other problematic issues, such as limited reserves, toxic emissions, waste disposal, excessive land usage, and high costs. One possible solution that can potentially have a large impact is nuclear fusion.

In order to increase electricity production and achieve an economic and environmentally friendly way of producing energy in the future, nuclear fusion is nowadays seen as a sustainable long-term solution. Firstly, fuel reserves are abundant. In fact, there are 34 grams of deuterium (D) for every ton of water, which means that it is available at least one million times more than all fossil fuels. Tritium (T) is not found in nature, but can be obtained by bombarding lithium with neutrons. The limiting reactant is lithium. Lithium is found in water in the ratio of 0.7 grams per ton of water and this proportion increases in the Earth’s crust to 20 ppm. According to geological studies, there are approximately 20 000 years of inexpensive Li available on Earth (assuming total world energy consumption at the present rate) [4]. In the meantime, deuterium-deuterium (DD) reactors will be developed before lithium is exhausted. Secondly, the cost of deuterium is low: from 0.1% to 1% the cost of fossil fuels, per unit of energy produced. Thirdly, the periods of material activation extend for approximately 100 years, extremely less than those reached in nuclear fission reactors [5]. The fourth advantage is the intrinsically safety operation of nuclear fusion devices of as there is no possibility of releasing radioactive waste to the atmosphere. Furthermore, the amount of fuel used for the reaction to occur is restricted to the burnt fuel: there is no chain reaction taking place.
1.2 The ITER Tokamak

ITER (International Thermonuclear Experimental Reactor) will be the largest tokamak in the world and is currently under construction in Cadarache (southern France) with the support of Europe, Japan, Russia, USA, China, India and South Korea. ITER will demonstrate the scientific and technological feasibility of obtaining fusion energy by magnetic confinement.

The predecessor of ITER is the Joint European Torus (JET), shown in Figure 1. JET is a non-superconducting tokamak and was the first to produce fusion power reaching a peak of 16 MW. ITER will use superconducting magnets instead to carry higher current and produce stronger magnetic fields while consuming less power at a reduced cost. The production of 500 MW of power will overcome the 50 MW input power needed in the processes of heating and confinement. It will also hold 9 times the plasma volume of JET in order to reach conditions of energy multiplication. The first plasma for ignition and power with deuterium-tritium (DT) in ITER may start at the end of 2025 [6].

![Figure 1: Internal view of the JET tokamak superimposed with an image of the plasma [7].](image)

The main characteristics of ITER are summarised in Figure 2 and Table 1. To guarantee safety and reliability at a reasonable cost, a compromise is taken between physical requirements, such as stability and plasma confinement, and engineering constraints. The main engineering constraints are the size of the superconducting coil and their supporting structures, the high neutron and heat fluxes in the first wall of the vacuum vessel and in the divertor, the need for remote handling for maintenance and intervention procedures, cryogenics and vacuum systems and the breeding technology.

Superconducting magnets will initiate, confine, shape and control the ITER plasma from 51 Gigajoules (GJ) of magnetic energy. The 10000 tonnes of magnets become superconductive at 4 Kelvin and are made from niobium-tin (Nb$_3$Sn) and niobium-titanium (NbTi). The magnet system comprises toroidal field (TF) coils, a central solenoid (CS), external poloidal field (PF) coils and correction coils (CC). The 18 D-shaped TF magnets confine the plasma particles, the CS is in charge of inducing current into the plasma, the six ring-shaped PF coils shape the plasma and pull the plasma away from the walls, and
the 18 CC located between the TF and PF coils will compensate field errors caused by geometrical deviations due to manufacturing and assembly tolerances. In-vessel coils consist of two non-superconducting coil systems (Vertical Stability) that provide additional plasma control capabilities and 27 coils (Edge-Localized Modes) that create resonant magnetic perturbations in the plasma so that certain types of plasma instabilities are avoided.

Figure 2: The ITER tokamak, adapted from [8].

<table>
<thead>
<tr>
<th>Total Fusion Power</th>
<th>500 MW (700 MW)</th>
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<tr>
<td>Q = fusion power/additional heating power</td>
<td>≥10</td>
</tr>
<tr>
<td>Average 14 MeV neutron wall loading</td>
<td>0.57 MW/m² (0.8 MW/m²)</td>
</tr>
<tr>
<td>Plasma inductive burn time</td>
<td>≥400 s</td>
</tr>
<tr>
<td>Plasma major radius (R)</td>
<td>6.2 m</td>
</tr>
<tr>
<td>Plasma minor radius (a)</td>
<td>2.0 m</td>
</tr>
<tr>
<td>Plasma current (I_p)</td>
<td>15 MA (17 MA*)</td>
</tr>
<tr>
<td>Toroidal field at 6.2 m radius (BT)</td>
<td>5.3 T</td>
</tr>
<tr>
<td>Plasma volume</td>
<td>837 m³</td>
</tr>
<tr>
<td>Plasma surface</td>
<td>678 m²</td>
</tr>
<tr>
<td>Installed auxiliary heating/current drive power</td>
<td>73 MW**</td>
</tr>
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</table>

Table 1 – Main plasma parameters and dimensions [9]. (*) The machine is capable of a plasma current up to 17MA, with the parameters shown in parentheses. (**) A total plasma heating power up to 110MW may be installed in subsequent operation phases.
The stainless steel vacuum vessel acts as a safety containment barrier and houses the fusion reactions. The 440 blanket modules shield the vacuum vessel and external machine components from heat and high-energy neutrons produced during the fusion reaction. The energy carried by the neutrons is transformed into heat energy and collected by the water coolant, which in a future power plant will be used for electrical power production. The refrigeration system and the regeneration of consumed tritium will be verified in limited areas of the tokamak, in experimental modules of the blanket but not in the total coverage of the wall. In addition, the stainless steel cryostat encloses the vacuum vessel and ensures a super-cool vacuum environment for the superconducting magnets and the vessel.

The divertor is located at the bottom of the vacuum vessel and has 54 properly refrigerated cassette assemblies that deviate the charged particles produced in the fusion reaction from the walls. There are ports of access to the plasma for heating, diagnostics and tests. Like the blanket, the heat in this component is removed by active water cooling.

1.3 The Plasma Position Reflectometry (PPR) System

ITER requires fusion diagnostics to provide key measurements of the plasma and the first wall parameters in order to achieve machine protection, basic and advanced plasma control and perform physics studies. In other words, a good diagnostics system alerts and prevents damages in the tokamak as plasma can cause enormous disruptions if it impacts the first wall. In addition, diagnostics are useful to optimize plasma performance while in operation and validate physical models on the plasma behaviour under different operational conditions.

The Plasma Position Reflectometer (PPR) is a diagnostics system which comprises of five fully independent reflectometers located in gaps 3, 4, 5, and 6, distributed poloidally and toroidally in the vacuum vessel (See Figure 3). The purpose of Specific Grant 04 (SG04) of the F4E Framework Partnership Agreement 375 (F4E-FPA-375) consists in executing the R&D and prototyping activities for the components of gaps 4 and 6 of the PPR system to be installed inside the vacuum vessel. This Thesis is focused on the PPR system located in gap 4.

Figure 3: Location of gaps in the ITER tokamak showing a poloidal cut in (a) and (b) and a toroidal cut in (c) [10].
The system of gap 4 is located in sector 9 and accesses the ITER vacuum vessel through the bottom part of the port extension of upper port 01. The antennas are installed in the low-field side in the gap between the blanket modules (BM) #11 and #12 and attached to a 90-degree bend whose support is bolted to a baseplate welded to the vessel wall. Straight and curved sections of rectangular waveguide are used to route the microwaves between the 90-degree bend and one of the lower feed-outs of upper port 01. All these components are made of ITER-grade steel 316L(N)-IG. In order to reduce ohmic losses, the inner surfaces of the waveguides are coated with a copper layer (15-25 µm) [11].

This diagnostics system comprises antennas, waveguides (see Figure 4) and microwave electronics, together with real-time analysis software. A radio frequency signal in the range 15 – 75 GHz sent and received by the antennas and waveguides will be assessed by microwave electronics and real-time analysis software to determine the distance between the plasma and the tokamak wall and the density profile at the plasma edge. The parameters will be introduced into the plasma control system to keep the plasma stable without any disruption, preventing it from stopping the nuclear fusion process [12].

![Figure 4: PPR antennas and waveguides [11].](image)

The technique, known as broadband microwave reflectometry, uses electromagnetic waves that are reflected at density layers (dependent on the wave’s frequency) where its local refractive index goes to zero. The position of the density layer in the plasma is known from comparing the phase of the reflected wave with a reference wave. When the frequency of the probing wave is varied, different density layers are probed, which allows to reconstruct the electronic density profile.

Antennas and waveguide systems are suitable for ITER’s severe environment, requiring reduced machine access. Another important characteristic is the possibility of accommodating itself in a restricted space in the tokamak.
1.4 Problem Statement

The in-vessel components of the PPR system will be directly exposed to high levels of ionizing radiation: 14.1 MeV neutrons generated from the fusion reaction and prompt gamma photons generated from nuclear interactions in the surrounding materials. The aim of this Thesis is to contribute to the study of the effect of the nuclear loads in the PPR components.

The Thesis starts with chapter one as an introduction where nuclear fusion is described as a promising solution to fulfil future consumption of energy. The ITER tokamak aims at proving the feasibility of nuclear fusion for energy production. The PPR system is part of the ITER’s diagnostics systems and its integrity can be compromised by the effects of ionizing radiation.

Chapter two shows the theoretical fundamentals needed to understand the Thesis. It provides a theoretical background on physics and mechanics: fusion reaction, neutron and photon interactions with matter and the Monte Carlo and Finite Elements methods.

Chapter three shows the used methodology. In a first stage, a shielding sphere is described and it is shown how to carry out the thermal analysis in ANSYS. Finally, a MATLAB interface is done between MCNP6 and ANSYS to obtain the temperature distribution in the shielding sphere as a function of different parameters. In a second stage, the preliminary work already carried out for the PPR system is described. MCNP6 is a state-of-the-art Monte Carlo simulation program employed in the nuclear analysis performed for ITER. It allows the calculation of energy deposition and neutron and photon fluxes. The nuclear library FENDL 3.1 and the cross section processing program NJOY are used in conjunction with MCNP6 to calculate the DPAs in the PPR components.

In chapter four, the results are presented. The first part includes the shielding problem, where neutron and photon fluxes, power density and temperature distribution are studied. The PPR system is then analysed according to the total heat loads and the DPAs. After calculating the DPAs, the analysis is supplemented by the results of a previously performed thermal analysis in order to assess the feasibility of the system and propose alternative configurations.

Chapter five presents the conclusions of this work, proposing alternative configurations and pointing out the future work.
2 FUNDAMENTALS

2.1 Controlled Thermonuclear Fusion

Nuclear fusion is the process in which two light atoms, such as hydrogen, fuse into a heavier element. Since the products of the reaction have less mass than the reactants, energy is released in the process. Even though fusion powers the sun and the stars through fusion processes such as proton-proton fusion, the carbon cycle and the triple-alpha process, the deuterium-tritium fusion reaction contained by magnetic confinement seems to be the most promising reaction for the production of nuclear fusion energy in a controlled environment on Earth [13]:

\[ D + T \rightarrow \alpha + n + 17.6 \text{ MeV}, \]  

(2.1)

where D is deuterium and T is tritium (see Figure 5). The controlled thermonuclear reaction is self-sustaining: the thermal energy output exceeds the input. The energy released is distributed in 3.5 MeV for the alpha particle (α) and 14.1 MeV for the neutron (n). Since the alpha particles are charged, they are confined by the magnetic field and do not escape. When the magnets are turned off, these helium nuclei can collide with the walls (they do not penetrate far and can be stopped by paper), recombine with some electrons, and return to being helium, an inert and harmless gas [14].

![Nuclear fusion reaction](image)

Figure 5: Nuclear fusion reaction [15].

On the other hand, neutrons need to be studied as they are highly energetic (they carry 80% of the total released energy) and will reach the components surrounding the plasma chamber, mainly the blanket, where energy deposition takes place. As these neutrons are captured in the blanket, they do not pose a threat to the public. The heat produced in the blanket will be removed from the reactor core by a primary coolant and may produce electricity. Neutrons are not stopped easily and are able to penetrate several metres into materials producing gamma rays, secondary particles and radioactive nuclei. Microscopic changes are created in the material structure which may cause degradation of physical and mechanical properties [16].

At the same time, neutrons in the blanket can be used to breed tritium by bombarding lithium. ITER will test mockups of breeding blankets, called Test Blanket Modules (TBM), in a real fusion environment.
Within these test blankets, viable techniques for ensuring tritium breeding self-sufficiency will be explored for future use in nuclear fusion power plants [17]. The following reactions may occur in order to obtain tritium:

\[
\text{Li}_3^6 + n \ (\text{slow}) \rightarrow \alpha + T + 4.8 \text{MeV} \tag{2.2}
\]

\[
\text{Li}_7^3 + n \ (\text{fast}) \rightarrow \alpha + T + n - 2.5 \text{MeV} \tag{2.3}
\]

In order to overcome the electrostatic forces for deuterium and tritium to fuse, a temperature of 150 million °C is required (10 times more than the temperature of the sun). The temperature is such that the kinetic energy of the nuclei is sufficient to overcome the Coulomb forces, until they become close enough to be acted upon by the nuclear forces. At this ignition temperature, the fuel becomes completely ionized. In other words, the medium consists of free electrons and atoms lacking some or all of the orbiting electrons, constituting what is called plasma.

Approximately one in every million collisions produces fusion, while the remaining are elastic collisions. Hence, a confined medium is needed so that the nuclei cannot escape and can collide more often. Another scientific challenge is to confine the plasma above the critical ignition temperature during a certain amount of time, called the confinement time. The energy confinement time is defined as a function of the global plasma energy content, \( W \), and the applied total heating power, \( P \) [18]:

\[
\tau_E = \frac{W}{P - \frac{dW}{dt}} \tag{2.4}
\]

The energy confinement time can be improved by reducing the losses and instabilities in the plasma, which can be achieved by employing diagnostics and advanced control techniques. Fritz Wagner observed a radical growth of confinement time at the tokamak ASDEX in 1982 and managed higher energy stored in the plasma, which was soon to be called H-mode [19]. However, a new instability type called Edge Localized Mode was observed in H-mode plasma [20]. During an ELM instability, a bunch of plasma particles is thrown from the plasma to the chamber wall, resulting in low plasma densities. Energetic particles hitting the chamber wall also reduce a chamber wall durability and damage sensitive diagnostic systems. Consequently, one of the functions of the Plasma Position Reflectometry system consists in measuring the edge plasma region with high temporal resolution.

Magnetic confinement seeks to increase the time that ions spend close to each other in order to increase the probability of fusion reactions to occur, whereas inertial confinement looks for a rapid fusion of nuclei for them to not move apart. The latter uses a tiny deuterium-tritium pellet and, by means of laser or ion-beams high energy influx, evaporates the outer layer of the pellet producing collisions which drive part of the pellet inward forming a surrounding plasma envelope. When the DT fuel in the core is compressed to a density of more than \(10^{30}\) particles/m\(^3\) in a time interval of \(10^{-11}\) to \(10^{-9}\) seconds, the ions do not separate because of their own inertia and the fuel ignites quickly, yielding many times the input energy. This process is illustrated by Figure 6.
Figure 6: Inertial confinement [20].

Figure 7 shows that magnetic confinement can be achieved with an energy confinement time longer than one second in a very low density plasma. The plasma consists of a gas of charged particles that experience electromagnetic interaction and can therefore be confined by a magnetic field of a particular geometry.

For magnetic confinement, a solenoid would be the simplest configuration, but the created field would consequently lose ions and electrons radially. The most common solution is to eliminate the ends altogether by bending the field lines around to close themselves. Among the different configurations, the tokamak features the best results for confinement. The tokamak (acronym of Russian words: TOroidal'naya Kamera s MAgnitnymi Katushkami) was first developed in the 1950’s by soviet physicists A. D. Sacharov, I. J. Tamm and L. A. Artsimovich [21][22]. Instead of using gravitational forces like in
the stars, the use of magnetic fields, which confine the plasma in the torus chamber, as shown in Figure 8, allows to reach the appropriate conditions for fusion.

![Diagram of Tokamak coil system, magnetic and toroidal fields and the resulting plasma confinement](image)

**Figure 8:** Tokamak coil system, magnetic and toroidal fields and the resulting plasma confinement [22].

From the point of view of the neutronics, which will be the main topic of this Thesis, the inertial confinement features neutrons of 12 MeV, instead of the 14.1 MeV neutrons of high density plasmas.

The amount of energy created relies on particles colliding and fusing. The greater the density, the more the particles collide and the higher the probability of fusion. The density reached in stellar interiors are of the order of $10^{33}$ particles/m$^3$ at a temperature of $3 \times 10^7$ K, while metals have a density of approximately $10^{28} - 10^{29}$ particles/m$^3$ and air of $2.7 \times 10^{25}$ molecules/m$^3$ in standard conditions. Gravitational confinement is therefore defined as a type of confinement occurring in the sun and the stars whereby gravity holds the plasma nuclei close enough together to fuse [23].

The Lawson criterion provides the condition under which efficient production of fusion energy is possible. Basically, it uses the electron density and the energy confinement time [24]. For the deuterium-tritium reaction:

$$n\tau_E \geq 1.5 \times 10^{20} \frac{S}{m^3}$$ (2.5)

Technologically, it is still necessary to prove the vast majority of the necessary technologies for a fusion power plant.

**2.2 Mechanisms of Nuclear Interaction**

Nuclear interactions can be represented as

$$a + X \rightarrow Y + b,$$ (2.6)
where a is the incoming particle or light element that acts as a projectile, X is the target nucleus, Y is the resultant nucleus and b is the outgoing particle. It can be simplified in the form of X(a,b)Y [25]. Some examples are:

\[ ^{2}\text{He} + ^{13}\text{N} \rightarrow ^{17}\text{O} + ^{1}\text{H} \]  
\[ ^{3}\text{n} + ^{10}\text{B} \rightarrow ^{7}\text{Li} + ^{4}\text{He} \]  

(2.7)  
(2.8)

Every nuclear interaction must obey the following laws [26]:

- Conservation of nucleons: the total number of nucleons before and after a nuclear reaction is not changed;
- Conservation of charge: the sum of the charges of all particles involved in the reaction before and after must be preserved;
- Conservation of linear and angular momentum: the total momentum of interacting particles before and after the reaction is not changed;
- Conservation of energy: energy, including the rest mass energies of particles, is not changed by a nuclear reaction.

The energy of the reaction is represented as follows:

\[ Q = (M_{n} + M_{x} - M_{y} - M_{b}) \times c^{2} \]  

(2.9)

If \( Q > 0 \), the reaction is exothermic and some of the nuclear mass is converted into kinetic energy. If \( Q < 0 \), the reaction is endothermic and the kinetic energy is converted into mass and hence there is a net decrease of the total kinetic energy of the particles. The velocity at which a 14.1 MeV neutron is emitted in a fusion reaction is

\[ v = \frac{2 \times E}{M_{n}} \approx 52 \times 10^{6} \text{m/s} \]  

(2.10)

**2.2.1 Neutron Interactions with Matter**

Due to their lack of charge, neutrons cannot interact through Coulomb forces with charged particles, and therefore they are not stopped in the ITER’s tokamak by electromagnetic forces. For that reason, they travel much larger distances in the materials than protons or electrons. For instance, the mean free path, which is the average distance travelled by a moving particle between successive collisions, of a neutron of 2 MeV in water is 3.2 cm [27].

Neutrons can be separated mainly into three categories according to their energies: Thermal (E~0.025 eV), epithermal (0.025 eV <E<100 keV) and fast neutrons (E>100 keV) [28]. In addition to the energy classification, the neutron can be characterized by its De Broglie wavelength, calculated as:

\[ \lambda = \frac{h}{p} = \frac{h}{\sqrt{2 \times m_{n} \times E}} \equiv \frac{2.86 \times 10^{-9}}{\sqrt{E(eV)}} (\text{cm}) \]  

(2.11)
where $\hbar$ is the Planck’s constant, $p$ is the momentum, and $m_n$ is the mass of the neutron. At decreasing energies, optical properties such as refraction and reflection of neutrons predominate in ordinary matter. As an example, for neutrons of 0.01 eV, the wavelength is approximately $10^{-8}$ cm, the value of the diameter of the atom; therefore these neutrons can be diffracted as X-rays do, but since they penetrate further they are suited for bulk materials [29]. As the energy increases, it is more common to point out neutrons as projectiles colliding with the individual particles that make up the nuclei. For fast neutrons of 1 MeV, the wavelength is in the order of magnitude of $10^{-12}$ cm, which is the magnitude of the diameter of the nucleus [30].

In order to understand neutron interactions with matter, the term cross-section is necessary. Normally measured in barns ($10^{-24}$ cm$^2$), the cross-section is the target area presented by a nucleus to an approaching neutron, measured as area on a plane normal to the motion of the neutron. Put simply, it is the area of projection of the actual nucleus on the plane, as shown in Figure 9 [31].

![Figure 9: Neutron cross sections and rate of reaction, adapted from [30].](image)

A more sophisticated definition for cross-section derives from the meaning of rate of nuclear reaction, $R$, which is proportional to the intensity of the neutron beam $I$ (neutrons/s.cm$^2$) and the number of atoms in the target per unit area $N$ (atoms/cm$^2$). The constant of proportionality is known as the microscopic cross-section $\sigma$ and quantifies the probability of any type of interaction that characterizes a nuclear reaction.

$$R = n \cdot v \cdot N \cdot \sigma = I \cdot N \cdot \sigma$$ (2.12)

The cross sections depend heavily on the kinetic energy of the incident neutrons [32]. Figure 10 shows the variation of the cross section of U-238 with the energy of the neutron. There are three main regions in the cross section plots. In the low-energy region, the cross sections vary approximately as $1/v$, being
ν the neutron speed [33]. Then there is the resonance region, where the cross sections exhibit a high sensitivity to slight variations in the energy of the incoming neutron, and the unresolved resonance region, where the resonances are so close to each other that they cannot be resolved [34]. In this specific case, the cross section describes the probability of undergoing radiative capture, described hereafter.

\[ \Sigma_t = N \cdot \sigma_t, \]  

(2.13)

where N is the atomic density of the material (atoms/cm\(^3\)). It has units of cm\(^{-1}\). Unlike microscopic cross sections, \( \Sigma_t \) is used to define the probability of interaction in a macroscopic volume instead of a single nucleus. The macroscopic cross section can be expressed as a function of the mean free path:

\[ \Sigma_t = \frac{1}{\lambda \text{ (mean free path)}} \]  

(2.14)

Furthermore, it can be used to describe the intensity of a neutron beam hitting a material as a function of the distance travelled in the material. Its intensity decreases with the distance according to the following exponential attenuation law:

\[ I(x) = I_0 \cdot e^{-\Sigma x} \]  

(2.15)
The total cross sections, $\sigma_t$ or $\Sigma_t$, can be obtained from the sum of the individual cross sections of the different interactions that a neutron can experience.

Neutrons are attenuated (reduced in energy and numbers) by two major types of interactions: scattering and absorption. Table 1 shows the different types of interactions of neutrons with matter:

<table>
<thead>
<tr>
<th>Scattering</th>
<th>Elastic (n,n)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Inelastic (n, n’ $\gamma$)</td>
</tr>
<tr>
<td>Absorption</td>
<td>Radiative capture (n, $\gamma$)</td>
</tr>
<tr>
<td></td>
<td>Capture with emission of charged particles (n,$\alpha$);(n,p);(n,d)</td>
</tr>
<tr>
<td></td>
<td>Fission (n,f)</td>
</tr>
<tr>
<td></td>
<td>(n,2n), (n,3n), spallation, etc.</td>
</tr>
</tbody>
</table>

Table 2: Different mechanisms of neutron interaction, adapted from [30]

Scattering events have the effect of changing the speed and the direction of the neutron and can be classified into elastic and inelastic scattering. In elastic scattering, represented in Figure 11, a neutron interacts with a nucleus and bounces off. Some of the kinetic energy of the neutron is transmitted to the nucleus of the atom, increasing its kinetic energy and slowing down the neutron. The incident neutron does not necessarily have to “touch” the nucleus; it may be scattered by the short range nuclear forces when it approaches close enough to the nucleus. This type of elastic scattering is called potential scattering. It occurs with incident neutrons that have an energy of up to 1 MeV, approximately, and may be modeled as a billiard ball collision between a neutron and a nucleus.

A more unusual type of elastic scattering is called compound elastic or resonance elastic scattering, which occurs if the kinetic energy of an incident neutron is just right to form a resonance. Then, the neutron may be absorbed, forming a relatively long-lived ($\sim > 10^{-17}$ sec) compound [35], but it is emitted afterwards.

Figure 11: Potential elastic scattering, adapted from [32].
The formation of a compound nucleus can be represented as

\[ {}_1^n + {}_2^X \rightarrow {}^{A+1}X^* \]  

(2.16)

This is more common in inelastic collisions whereby the compound nucleus decays through the emission of a neutron, but not necessarily the same neutron that hit the nucleus in the first place. Whereas in the elastic scattering reaction the total kinetic energy and momentum of the system is conserved, in inelastic scattering there is a loss of kinetic energy needed to produce an excited state of the nucleus, which decays to the fundamental state through the emission of gamma radiation (see Figure 12). There is no conservation of kinetic energy, as the variation of kinetic energy is used to leave the nucleus in the excited state.

![Diagram](image)

Figure 12: Inelastic scattering, adapted from [32].

If the mass of the nucleus is similar to the mass of the neutron, the neutron loses more energy than when it collides with heavy nuclei. The average energy loss of a neutron undergoing elastic scattering is:

\[ \text{Average energy loss} = \frac{2EA}{(A + 1)^2} \]  

(2.17)

where E is the kinetic energy of the neutron and A is the atomic weight of the target nucleus [36]. Therefore, light materials attenuate neutrons more effectively. That is why they are used in fission reactors as moderators in order to decrease the energy of the neutrons to be able to increase the cross the probability of inducing fission. As an example, Table 3 shows the average number of collisions required to reduce a neutron's energy from 2 MeV to 0.025eV through elastic scattering.

<table>
<thead>
<tr>
<th>Element</th>
<th>Atomic weight</th>
<th>Number of collisions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>1</td>
<td>27</td>
</tr>
<tr>
<td>Deuterium</td>
<td>2</td>
<td>31</td>
</tr>
<tr>
<td>Helium</td>
<td>4</td>
<td>48</td>
</tr>
</tbody>
</table>
Table 3: Average number of collisions required to reduce a neutron’s energy from 2 MeV to 0.025eV through elastic scattering [36].

The energy loss in inelastic scattering depends on the energy levels within the nucleus. Inelastic scattering is only possible when the neutron has sufficient energy to induce excited states in the nucleus.

In an absorption reaction, the neutron is absorbed into the nucleus of an atom. The nucleus may re-arrange its internal structure through the emission of one or more gamma rays (radiative capture), charged particles or one or more neutrons. If the nucleus emits only one neutron, then it is indistinguishable from a scattering event. When the target nucleus is fissionable, a fission reaction may occur, whereby the nucleus splits into two nuclei of intermediate masses (the mass of each nucleus is variable), emitting a variable number of neutrons in the process.

Radiative capture occurs at most neutron energy levels, but it is more probable at lower energies [37]. The following reaction, represented in Figure 13, takes place:

$$^{1}_0 n + ^2 X \rightarrow ^{4}_2 X^* \rightarrow ^{A+1}_2 X + \gamma$$  (2.18)

A gamma photon is emitted and the target nucleus is changed to a different isotope of the same element.

![Figure 13: Radiative capture, adapted from [38].](image)

Transmutation, which is the transformation of one element into another through a nuclear reaction, may occur when the compound nucleus emits a charged particle, as shown in Figure 14. An example of this type of capture is the following:

$$n + ^{10}_3 B \rightarrow ^{7}_2 Li + \alpha$$  (2.19)
The large absorption cross section of helium-3, uranium-235 and boron-10 for the production of charged particles with low-speed neutrons makes it appropriate for use in neutron detectors. Since only thermal neutrons are detected, most detectors feature moderators, such as hydrogen or deuterium. Note that hydrogen requires fewer collisions than deuterium in order to moderate the neutron. Despite the cost and the abundance of hydrogen or water, the use of deuterium can be used instead as it features a smaller absorption cross section for neutrons. The high absorption cross sections of boron and cadmium make them useful as thermal-neutron poisons [36].

When nuclear fission occurs, the compound nucleus formed with the absorption of a neutron is split into two lighter nuclei (fission fragments) releasing gamma radiation as well as a variable number of neutrons. An example of a fission reaction initiated by a thermal neutron is:

\[ n + ^{235}_{92}U \rightarrow ^{235}_{92}U^* \rightarrow ^{92}_{36}Kr + ^{144}_{56}Ba + 3n \]  

(2.20)

Figure 15 shows graphically the mechanism of nuclear fission, whereby a neutron encounters a nucleus and forms a compound nucleus. The compound nucleus then emits two fragments, gamma radiation and two neutrons in order to de-energize. The fission products are highly radioactive and decay through the emission of \( \gamma \) and \( \beta \) radiation [34].

\[ n + ^{235}_{92}U \rightarrow ^{235}_{92}U^* \rightarrow ^{92}_{36}Kr + ^{144}_{56}Ba + 3n \]
2.2.2 Photon interactions with matter

Electromagnetic radiation can be considered as a beam of photons with energy:

\[ E = h \nu \]  \hspace{1cm} (2.21)

Photons are neutral particles so they do not interact by Coulomb forces. If the energy of the incident photon is above 10 eV, then photons may undergo photoelectric and Compton effect and ionize matter directly [39]. However, photons are called indirectly ionizing radiation since most of the affected atoms in matter are ionized directly by the secondary beta particles, which come from the ejection of an electron from an atom at relativistic speeds [40]. The interactions of photons with matter that lead to the production of secondary beta particles are:

- Photoelectric effect
- Compton effect
- Pair production

The probability of photon interaction with matter depends on the incident energy of the photon \( E \) and the atomic number of the target \( Z \).

Table 4 shows that the cross section for photoelectric effect is higher for low energies of the incident photon and for heavy target nuclei. On the other hand, it is more probable for pair production to occur at higher energies.

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Cross section (barns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photoelectric effect</td>
<td>[ \sigma = k \frac{Z^n}{E^3} ] ( n ) between 3 and 5 depending on the energy of the photon</td>
</tr>
<tr>
<td>Compton effect</td>
<td>[ \sigma = k \frac{Z}{E} ]</td>
</tr>
<tr>
<td>Pair production</td>
<td>[ \sigma = k Z^2 (E - 1.022 \text{ MeV}) ]</td>
</tr>
</tbody>
</table>

Table 4: Dependence of the total cross section on the incident energy of the photon and the atomic number according to the main different mechanisms [27].
Figure 16 describes the dependence of the cross section on the energy of the incident photon for the case of lead, where $\tau$ is the photoelectric effect, $\sigma_{\text{INCOH}}$ is the incoherent (Compton) scattering, $\sigma_{\text{COH}}$ is the coherent scattering, $\kappa_n$ is the nuclear-field pair production, $\kappa_e$ is the electron-field production (triplet) and $\sigma_{\text{PH.N.}}$ is the nuclear photoabsorption. The different processes are explained hereafter.

Figure 16: Contributions of different effects to the total measured cross section in lead over the photon energy range between 10eV to 100 GeV [37].

The photoelectric effect is a process whereby a photon is absorbed by the atom it encounters. The photon transmits all its energy to an atomic electron. This electron is called photoelectron and escapes from the atom with a kinetic energy equal to the difference between the energy of incident photon and the binding energy of the atom $B$, which in turn is dependent on the atomic layer at which the electron is located:

$$E_e = h \nu - B \quad (2.22)$$

The Compton effect is equivalent to an inelastic collision, as part of the photon energy is transferred to the electron and a less-energetic photon bounces off, which means that it has lower frequency (or longer wavelength).

For a quantitative analysis, the laws of conservation of energy and momentum are used:

$$E_y + m_e c^2 = E_{y'} + m_e c^2 + E_e + B \quad (2.23)$$

$$\vec{p}_y = \vec{p}_{y'} + \vec{p}_e \quad (2.24)$$
where $E_{\gamma}$ is the energy of the incident photon, $E_{\gamma'}$ is the energy of the scattered photon, $E_e$ is the kinetic energy after the collision, $B$ is the binding energy of the electron and $m_e c^2$ is the energy equivalent to the mass of the electron at rest.

If the electron is considered as a free electron, then $B \approx 0$ and equation 2.25 can be simplified:

$$E_{\gamma} = E_{\gamma'} + E_e$$

After some operations, the difference in wavelength after and before scattering is obtained:

$$\Delta \lambda = \lambda' - \lambda = \lambda_c (1 - \cos \theta),$$

where $\lambda'$ is the wavelength of the scattered photon, $\lambda$ is the wavelength of the incident photon and $\theta$ is the angle formed between the scattered photon and the incident photon. Compton’s wavelength is represented by $\lambda_c$ and its value is:

$$\lambda_c = \frac{h}{m_e c} = 2.43 \times 10^{-12} = 0.0243 \text{ Å}$$

Coherent/Rayleigh/elastic scattering is a process by which photons are scattered by bound electrons and in which the atom is neither ionized nor excited. The photon loses only a negligible fraction of its energy, since the recoil is by the entire atom including the nucleus, rather than by an individual atomic electron as in the Compton effect [41].

Figure 17 shows the different mechanisms in a schematic way, where A is a photon that does not interact with matter, B shows the photon undergoing photoelectric effect and C and D represent the photon undergoing Rayleigh and Compton scattering, respectively.

![Photon interactions](image.png)

Figure 17: Photon interactions [42].
At higher energies – above \( \sim 10 \) MeV – pair production predominates. When the photon passes close enough to a heavy nucleus, it converts itself into an electron and a positron (the positron is the antiparticle of the electron, having the same mass but positive charge). The incoming photon energy must be above a threshold in order to create the pair: at least the total rest mass energy of the two particles, satisfying the expression

\[
E_{\gamma \text{min}} > 2 m_0 c^2 (1 + \frac{m_0}{M}) \tag{2.28}
\]

where \( m_0 \) is the rest mass of the particle or antiparticle and \( M \) is the mass of the nucleus [27].

If \( m_0 \ll M \) the minimum energy required to produce an electron-positron pair is

\[
E_{\gamma \text{min}} = 2 m_0 c^2 = 2 \times 0.511 \text{ MeV} = 1.022 \text{ MeV} \tag{2.29}
\]

Finally, positron annihilation may occur. It is the inverse process, in which the created positron is combined with an electron, producing two photons of 0.511 MeV each.

Processes of relatively minor importance are the electron-field production or triplet and the nuclear photoeffect. In the electron-field production, the atomic electron involved in this process is also ejected from the atom, giving rise to a trident signature including the created electron and positron. The nuclear photoeffect is the process in which the photon is absorbed by the atomic nucleus and one or more nucleons (neutrons and/or protons) are ejected [41].

### 2.3 The Monte Carlo Method

The Monte Carlo method describes physical systems and processes with stochastic behaviour, such as the interaction of radiation with matter, using probability theory and statistical methods. Specifically, the Monte Carlo method applied to radiation transport simulates individual particles and records aspects (tallies) of their average behaviour in order to obtain an approximate answer to the problem. The simulation of the different interactions which take place along the paths of the particles through matter is carried along according to theoretical physical models or experimental cross sections [34][30][43].

Some of the components for a simulation using the Monte Carlo method are:

- Probability Density Functions: The physical system or mathematical problem shall be described by the means of a set of probability density functions, which is a function \( f \) defined in the interval \([a,b]\) and has the following properties:

\[
1. \quad f(x) \geq 0 \quad \forall x \in [a,b] \tag{2.30}
\]

\[
2. \quad \int_a^b f(x) dx = 1 \tag{2.31}
\]

\[
3. \quad P(x_1 \leq x \leq x_2) = \int_{x_1}^{x_2} f(x) dx \tag{2.32}
\]
• Pseudo-random number generator: A source of pseudo-random numbers from a probability density function uniformly distributed between 0 and 1 is needed [44][45]. Even though pseudo-random number generators still exhibit periodicity (when a number is repeated the whole sequence is repeated), they feature sophisticated and efficient algorithms generated from an initial number, called the seed. The seed can be changed to produce different random number sequences. For example, when the pseudo-random generator is called, the seed can be extracted from the computer system clock.

• Error estimate: The error is proportional to $1/\sqrt{N}$, where $N$ is the number of histories and is inversely proportional to the computational time.

The name Monte Carlo arose from the analogy between the statistical sampling process based on the selection of random numbers with throwing dice in the gambling casino of the capital of Monaco. Due to increased computational capacity and need to solve problems of diffusion of neutrons, the Monte Carlo method became more relevant during the II World War. Nowadays, there are several radiation transport programs that use this method, such as [46]:

- EGSnrc and PENEOPE, appropriate for electron, positron and photon transport;
- GEANT4 and FLUKA, which can also simulate neutrons and many more types of particles;
- MARS, for thermal and stress analyses;
- PHITS and SHIELD, focused on the analysis of heavy ions;
- TRIM, for protons and heavy ions undergoing Coulomb interactions.

Monte Carlo N-Particle (MCNP) is another radiation transport program that applies the Monte Carlo method, developed by the National Laboratory Los Alamos in the United States. It is used to simulate neutron, photon and electron transport in arbitrary three-dimensional geometries. Furthermore, MCNP6 uses ENDF1 formatted data such as the FENDL (Fusion Evaluated Nuclear Data Library) libraries. These libraries feature point-wise cross section data for neutron transport, which means that there is no approximation or averaging in the cross section data. A very accurate description of neutron transport is thus attained [47].

The transport of a single particle can be described as a sequence of collisions, events, occurring at discrete spatial locations followed by the transition of the particle from one collision point to the next collision point. At collisions, the incoming particle direction and energy are changed, whereas during the transition between two consecutive collision points the energy and direction of the particle is maintained.

At first, MCNP creates a virtual particle according to the source specification written by the user: the energy, direction and starting position are specified. The distance to the next collision is sampled from

$$l = -\frac{1}{\Sigma_a}\ln(\xi)\ldots(2.33)$$

where $l$ is the distance to next collision in cm, $\Sigma_a$ is the total macroscopic cross section in cm$^{-1}$ and $\xi$ is a uniformly distributed random number between 0 and 1 [47]. Knowing the fractional composition of
each nuclide for a given material, MCNP uses the pseudo-random generator to determine all required physical parameters during the "life" of the particle (also called the **history** of the particle), such as: with which nuclide the particle will interact, the type of interaction the particle and the nuclide undergo (depending on the cross sections) and the direction and energy of emission of secondary particles.

Figure 18 shows how the history of a neutron is simulated in MCNP. The steps that the neutron follows during this history are the following:

1. In the first event, the neutron undergoes inelastic scattering. MCNP follows the path of the neutron first and then focuses on the secondary particles created. In other words, the photon created in this case is temporarily stored in memory until the neutron is "killed". The neutron is deflected through an angle determined from the scattering distribution which is stored in the nuclear data.
2. Then the neutron is absorbed. Concretely, the neutron undergoes an (n,2n) reaction. So the code creates two neutrons with particular energies and directions.
3. Neutron absorption takes place for one of the neutrons from the previous (n,2n) reaction.
4. The second neutron produced in the (n,2n) reaction is retrieved from memory and leaks from the system.
5. The photon produced in the inelastic scattering reaction is retrieved from memory and undergoes pair production.
6. Photon absorption takes place for one of the photons that are produced.
7. The other photon which is retrieved from memory and was created from the pair production reaction undergoes a scattering reaction.
8. The photon leaks from the system.

![Event Log](image)

**Event Log**

1. Neutron Inelastic Scatter
2. (n,2n) Reaction
3. Neutron Absorption
4. Neutron Leakage
5. Pair Production
6. Photon Absorption
7. Photon Scatter
8. Photon Leakage

Figure 18: Neutron interaction events in MCNP [48].
The three tallies used in this Thesis are the surface averaged particle flux \((F_2)\), the volume averaged particle flux \((F_4)\) and the heating or energy deposition tally \((F_6)\), shown in Eqs. 2.34, 2.35 and 2.36:

\[
F_2 = \frac{1}{A} \int dE \int dt \int dV \int d\Omega \ \phi(r, \Omega, E, t),
\]

\[2.34\]

\[
F_4 = \frac{1}{V} \int dE \int dt \int dV \int d\Omega \ \phi(r, \Omega, E, t),
\]

\[2.35\]

\[
F_6 = \frac{\rho a}{m} \int dE \int dt \int dV \int d\Omega \ \sigma_r(E) \ H(E) \ \phi(r, \Omega, E, t).
\]

\[2.36\]

where \(V\) is the volume of the cell in cm\(^3\), \(E\) is the energy of the particle in MeV, \(t\) is the time since the particle was created in shakes, \(\Omega\) is the direction vector, \(\phi\) is the angular flux of particles is cm\(^2\), \(r\) is the position of the surface, \(\frac{\rho a}{m}\) is the atom density per unit of mass of the cell in atoms/barn cm g, \(\sigma_r\) is the microscopic total cross section in cm\(^2\) and \(H(E)\) is the heating number in MeV/collision.

### 2.4 The Finite Element Method

The Finite Element (FE) method is a method for numerical solutions of field problems, which require determining the spatial distribution of one or more dependent variables [49]. The FE method consists of dividing the actual physical system into small subdomains or elements with finite degrees of freedom. The variable in each FE has the restriction of simple spatial variations described by, for example, second order polynomials. FEs are structured in the following way: points, termed as nodes, are connected by lines to form a mesh, which is the union of lines represented by a system of algebraic equations. These algebraic equations are created using integral formulations rather than difference equations and are to be solved while having nodal unknowns [50].

For a thermal FE analysis, the Fourier’s law is applied to the heat equation [51]:

\[
\frac{\partial}{\partial x} \left( k \frac{dT}{dx} \right) + \frac{\partial}{\partial y} \left( k \frac{dT}{dy} \right) + \frac{\partial}{\partial z} \left( k \frac{dT}{dz} \right) + Q_v = \rho c \frac{dT}{dt}.
\]

\[2.37\]

where \(k\) is the conductivity, \(T\) is temperature, \(Q_v\) is the internal heat generation rate per unit volume, \(\rho\) is the density, \(c\) is the specific heat capacity and \(t\) is time. The boundary conditions used for the different cases in the thesis are:

- **Specific temperature**

  \(T_s = T(x, y, z, t)\) on the surface (S) \[2.38\]

- **Radiation**

  \(q''_z n_x + q''_y n_y + q''_x n_x = E - aG\) on S, \[2.39\]
where \( q''_x, q''_y \) and \( q''_z \) are components of heat flow per unit area, \( n_x, n_y \), and \( n_z \) are the components of the normal unit vector to the surface, \( \alpha \) is the absorptivity, \( G \) is the incoming heat flow per unit area named irradiation and \( E \) is the emissive power which is expressed by:

\[
E = \varepsilon \sigma T^4,
\]

(2.40)

where \( \varepsilon \) is the emissivity and \( \sigma \) is the Stefan-Boltzmann constant.

- Steady-state regime:

\[
\frac{\partial T}{\partial t} = 0
\]

(2.41)

Eq. 2.37 can be rewritten as follows after applying Fourier’s Law, the Galerkin weighted residual method [52] and the divergence theorem [53] to the components of the heat flow per unit area:

\[
\int_V \rho c \frac{\partial T}{\partial t} N_i dV - \int_V \left[ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial y} \frac{\partial N_j}{\partial z} \right] \{q\} dV = \int_V Q_v N_i dV + \int_S \{k[B][T]\}^T \{n\} N_i dS - \int_S (\varepsilon \sigma T^4 - \alpha G) N_i dS
\]

(2.42)

where \( \{n\} \) is the outer normal to the surface of the body and \( [B] \) is the matrix containing the partial derivatives of the shape functions \( N_i \), which are used for interpolation of temperature inside a FE. Boundary conditions (2.38) and (2.39) are inserted. Note that as vacuum in the vessel is present, convection is neglected.

Hence, Eq. 2.42 after assembly becomes:

\[
[C]\{\dot{T}\} + ([K_c] + [K_{rad}])\{T\} = \{R_T\} + \{R_{rad}\} + \{R_Q\},
\]

(2.43)

where \( [C] \) is the general global specific heat, \( ([K_c] + [K_{rad}]) \) are the conductivity matrices, and \( \{R_T\} + \{R_{rad}\} + \{R_Q\} \) are vectors for the global heat flux, radiation and heat generation, respectively, expressed as:

\[
[C] = \int_V \rho c [N]^T [N] dV
\]

\[
[K_c] = \int_V k [B]^T [B] dV
\]

\[
[K_{rad}] = \int_S \varepsilon \sigma T^4 [N] dS
\]
\[
[R_P] = \int_{S} (k[B](T))^T(n)[N]^T dS
\]  
\[
[R_{rad}] = -\int_{S} \alpha G[N]^T dS
\]  
\[
[R_{Qv}] = \int_{V} Q_v[N]^T dV
\]  

For a steady rate analysis, the governing equation after applying Eq. 2.41 is:

\[
([K_c] + [K_{rad}])[T] = \{R_T\} + \{R_{rad}\} + \{R_{Qv}\}
\]  

This formulation is adopted in the FE analysis conducted in this thesis.
3 METHODOLOGY

3.1 Shielding Sphere

3.1.1 MCNP PROCEDURE

A simplification of the real problem in ITER is done for practical and training purposes to deepen the knowledge about shielding materials. The shielding sphere shows the procedure to obtain the power density by using the Monte Carlo method in MCNP6 and the temperature distribution by using the Finite Element method in ANSYS. In this case, water and lead will be the selected shielding materials for the homogeneous source of 14 MeV neutrons. Moreover, they serve as a model for the innovative interface MMA.

At first, a sphere of radius 400 cm (cell 1) is defined as an approximation of the radius size of the plasma (neutron source). Cell cards indicate the cell number followed by the material number and the density among other information. The mass density of the cell starts with a negative sign to indicate that it is in g/cm$^3$. No density is entered for a void cell (written as 0 after the cell number). In the case of lead, the density is 11.34 g/cm$^3$ while water has a density of 1 g/cm$^3$. The cells are the areas defined by the surfaces that are shown in the next section.

1 0 -1 $source
2 1 -11.34 1 -2 $8 shielding layers
3 1 -11.34 2 -3
4 1 -11.34 3 -4
5 1 -11.34 4 -5
6 1 -11.34 5 -6
7 1 -11.34 6 -7
8 1 -11.34 7 -8
9 1 -11.34 8 -9
10 1 -11.34 9 -10
11 2 -1 -11 $water sphere
12 0 11 10 -12 $cell around the water sphere
13 0 12 $outer space

The surfaces are concentric spheres of different radii centred in the origin (So). The shielding layers (cells) have a width of 40 cm and from surface 6 outwards they have a width of 75 cm.

C Surface cards
1 So 400 $sphere source
2 So 440 $shielding layers
3 So 480
4 So 520
5 So 560
6 So 600
7 So 675
8 So 725
9 So 800
10 So 875
Data cards are needed to define the type of particles, problem materials, radiation sources and how results are to be scored (or tallied), amongst others. The variables are specified in Table 5.

Tally cards are then used to specify what you want to learn from the Monte Carlo calculation. F2, F12, F4, F14 and F6 are used for neutron (N) or photon (P) fluxes (tallies of type 2 and 4) and energy deposition (tallies of type 6). Energy bins (E2, E12, E4 and E14) are used to subdivide the total flux into energy bins [54]. Material cards are shown in the form ZZZAAA, consisting of the proton number and the mass number respectively and followed by the nuclide fraction, which can be left without normalisation. NPS terminates the execution of MCNP and is followed by the number of histories to transport. In other words, MCNP will terminate after NPS histories. Finally, a mesh tally is specified to plot the neutron fluxes in a 2D mesh plot. A multiplier factor is used to normalize the results to n/cm²s.

<table>
<thead>
<tr>
<th>MCNP commands</th>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SDEF</td>
<td>POS</td>
<td>Reference point for positioning sampling</td>
</tr>
<tr>
<td></td>
<td>RAD</td>
<td>Radial distance of the position from POS in cm. If the value is prefixed by a D, then the position will depend on the SI and will be sampled using probabilities entered on the associated SP card.</td>
</tr>
<tr>
<td></td>
<td>CEL</td>
<td>Cell number</td>
</tr>
<tr>
<td></td>
<td>ERG</td>
<td>Energy of the source particle in MeV</td>
</tr>
<tr>
<td></td>
<td>PAR</td>
<td>Type of source particle</td>
</tr>
<tr>
<td>SI</td>
<td>Source information: Range of the radial (indicated by SP) sampling.</td>
<td></td>
</tr>
<tr>
<td>SP</td>
<td>Source probability: -21 is the source probability function under the power law ( p(x) = c</td>
<td>x</td>
</tr>
</tbody>
</table>

Table 5: Source input information, obtained from [54] and [55].
C Data cards
mode n p
PRINT
IMP:N 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0
SDEF pos=0 0 0 rad=d1 cel=1 erg=14 par=N
SI 1 0 400 $ radial sampling range: 0 to Rmax
SP1 -21 2 $ weighting for radial sampling: here r^2
F2:N 2 3 4 5 6 7 8 9 10 $average neutron fluxes across each shielding surface
E2 1e-5 100log 20 $from 10 eV to 20 MeV takes log spacing
F12:P 2 3 4 5 6 7 8 9 10
E12 1e-3 100log 20
F4:N 11 $neutron flux across the water sphere cell
E4 1e-5 100log 20
F14:P 11
E14 1e-3 100log 20 $Energy photons
F6:N,P 2 3 4 5 6 7 8 9 10 $Energy deposition across each shielding cell
M1 82000 1 $Natural lead
M2 1001 2 8016 1 $Water
NPS 1000000
tmesh
rmesh31:n FLUX
cora31 -1000 99i 1000
corb31 -400 4i 400
corc31 -1000 99i 1000
demd
fm31 1.97e19

3.1.2 TRANSITION TO ANSYS

For the thermal analysis, the same geometry applied to MCNP6 is created with SolidWorks. First, half a sphere of 420 cm radius is modelled. The piece is then extruded with a smaller sphere of 400 cm radius, as shown in Figure 19.

The operation is repeated for all the outer semi-spheres. Finally, the ensemble of the pieces was made. Figure 20 shows two pieces of different width picked from the final semi-sphere.

The geometry is used as input in ANSYS and a superficial temperature and the internal heat generation in W/m³ obtained from MCNP6 were applied as boundary conditions.
Figure 19: Half a hollow sphere in SolidWorks.

Figure 20: Ensemble of pieces created in SolidWorks.
3.1.3 ANSYS PROCEDURE

In this section the methodology used in ANSYS Workbench and APDL are introduced. Note that the power density is input in ANSYS as internal heat generation. However, ANSYS works with W/m$^3$, and therefore a change in units from W/cm$^3$ is necessary, by simply multiplying by $10^6$.

3.1.3.1 ANSYS Workbench

In the Toolbox located at the left side of the window, Steady-State Thermal or Transient Thermal is chosen depending on the type of analysis required. Then a small window appears which initially contains a default list of steps to follow for obtaining the solution of the problem:

1. Engineering data: The material is selected if seen in the list. Otherwise, a material is chosen from the menu of Engineering Data Sources, shown in Figure 21:

   ![Engineering Data Sources](image)

   Figure 21: Engineering Data Sources to use new materials.

   Properties may be changed according to the requirements needed for the analysis.

   2. The Geometry is created in SolidWorks, saved in the STEP format and imported to ANSYS Workbench.

   3. In the Model option, a new window is opened and, following the Outline, a component is chosen and a material is assigned in the window below to each component by clicking on the field that appears in yellow, as shown in Figure 22.
After finishing with the geometry, the system is to be meshed as shown in Figure 23.

4. On top of the outline list, boundary conditions such as temperature at the surface and internal heat generation are selected and applied to each of the bodies.

5. The solution of the thermal analysis is finally achieved.

3.1.3.2 ANSYS APDL

Another way of obtaining similar results is by using the APDL. Even though different skills are required, the advantage is that it reduces the time needed to parametrize the FE model and performed the FE analyses. Figure 24 shows the main steps that were followed:
1. In Preferences there are options for thermal, structural, ANSYS fluid and electromagnetic analysis. Thermal analysis is selected.

2. In Preprocessor, the steps followed were:
   a. Select the FE
   b. In Material Props:
      i. Checking the units.
      ii. Selecting the material models and adding a model for each component.
      iii. Assigning a value for the thermal properties, which are known and available in the list presented in Figure 25.

   c. Creating a model. Some available operations are: extrude, add and overlap areas.

   d. Meshing:
      i. Picked volumes are selected and for each volume an element type is attributed.
      ii. In the MeshTool, the size of the mesh can be altered and all the volumes are selected and meshed.
e. If needed, in Numbering Ctrls, nodes can be merged.

f. Applying boundary conditions (Loads).

3. Under the option of Solution, Solve is clicked.

4. In Postprocessor, results were read and plotted.

The code for these steps can be introduced in the main bar and can be obtained by clicking on File > List > Log File.

3.1.4 MMA INTERFACE

A MATLAB-MCNP6-ANSYS interface was implemented to automatically input data such as: conductivity and density of the material, composition of the shielding material, source intensity and temperature in the outer layer. The aim of the interface is to be able to obtain the distribution temperature (i.e. maximum temperature) of the shielding sphere automatically, i.e. without changing the MCNP6 and ANSYS input files by hand. In this way, it is possible to perform a thermal analyses of a neutron source surrounded by different shielding materials.

Annex I shows the MCNP6 code used for the shielding sphere. Cell cards include the definition of the source and the eight shielding layers are rewritten in MATLAB code (annex III), introducing the density of the material used as shielding. Surface and data cards are also used from the MCNP6 shielding sphere bearing in mind the modifications needed for the multiplier factors in order to normalise results for the F4 and F6 tallies. The material card is then defined as ZZZAAA 1, where ZZZ is the proton number, AAA is 000, standing for the natural isotopic composition of the element, and 1 is the nuclide fraction.

With the MATLAB code, MCNP6 runs and particular lines of the output file (‘run_o’) are read and used as input data for ANSYS. Specifically, the lines are values of heat generation due to neutron irradiation, which is known as power density (in W/m³) in MCNP6. The input data is completed by introducing the variables of conductivity and density of the material, and the temperature in the outer layer as a boundary condition. Annex II shows the two methods of implementing the problem (manually or in batch mode).

3.2 PPR

3.2.1 PRELIMINARY WORK

Figure 26 shows a plane (y=0) of the reference MCNP model provided by F4E before the beginning of this work. This reference model, an effort of several institutions worldwide coordinated by the ITER Organization (IO), is extremely detailed, featuring more than 350,000 lines of MCNP code. Making changes to this model is therefore a difficult task, mainly due to the time it takes to visualize a plane in
the MCNP geometry plotter. Additionally, the location of gap 4 is particularly challenging, since it is tilted in the x, y and z directions, and the MCNP plotter only allows the visualization of 2D geometries.

Figure 26: Sectional cut of the MCNP reference model (y=0) [11].

Figure 27 shows the location of gap 4 in the reference model before the PPR components were created and implemented. It is clearly seen that there was space reserved in the model for the insertion of the PPR components. The reference model was modified as required to introduce some additional features,
such as the cut-outs in the blanket modules to accommodate the antenna assembly and provide access to the plasma \[11\].

Figure 27: Zoom for location of gap 4 in the MCNP reference model (plane defined by basis vectors $(706.2, 240.3, 0.0)$ and $(0.0, 0.0, 1.0)$) \[11\].

To produce the new MCNP to be used in the nuclear analysis of the PPR in-vessel components of gap 4, the CAD models of gap 4 available in ITER's ENOVIA database (where all the ITER CAD models are stored) were converted into a simplified neutronics CAD model. The simplifications involved the removal of spline surfaces, fillets and screws while preserving approximately the same volumes and masses of the components. The simplified neutronics CAD model was then divided into separate cells. As they are closer to the plasma, the parts of the antennas were divided into smaller cells (see Figure 28), which allows a more detailed calculation in the elements exposed to higher radiation doses. Finally, the simplified neutron CAD model was converted to the STEP format in order to be edited in ANSYS SpaceClaim and converted in the CAD based modelling program MCAM \[56\] to the MCNP input format \[11\].

Figure 28: In-vessel components of the PPR system. Left: Simplified neutronics CAD model. Right: Detail of the simplified neutronics CAD model \[11\].
The result of the integration of the PPR in-vessel components of gap 4 into the MCNP reference model provided by IO is represented in Figure 29. Apart from the insertion of the antennas and waveguides, a cut was introduced in the top of blanket module #12, so that the antennas are facing the plasma directly [11]. The model thus created was employed in this Thesis to perform the Monte Carlo simulations of the system. The heat loads had in the system had already been calculated; they are reproduced in this work and complemented with neutron and photon flux calculations, which are later used (the neutron fluxes) to estimate the DPAs in all the elements of the system.

![Figure 29 - Sectional cut of the final MCNP model, featuring the PPR components of gap 4.](image)

### 3.2.2 MCNP Procedure

The volumes and masses of each element of the PPR system, retrieved from the CAD models, are shown in Table 6 (it is important to notice that cell 12230 features a higher mass than is apparent in Figure 28, as it extends beyond what is shown in the Figure). The differences in volume of the CAD models (from the model available in the ITER database to the simplified model), were kept below 0.1% up to cell number 133414. For the remaining cells, the cross sectional surface area of the waveguides was kept unchanged between the two CAD models while differences in volume are not possible to compare as significant changes were done to the models.

From the input file, it has been checked that the mass density of the material used for all the cells of the PPR system, which is SS316L(N)-IG, is 7.93 g/cm³, indicated by a negative sign for mass density in the cell cards.
\begin{table}
\centering
\begin{tabular}{ccc}
Cell Number & Volume (cm$^3$) & Mass (g) \\
133401 & 2.46 & 19.49 \\
133402 & 2.46 & 19.49 \\
133403 & 2.33 & 18.51 \\
133404 & 2.33 & 18.51 \\
133405 & 2.21 & 17.54 \\
133406 & 2.21 & 17.54 \\
133407 & 1.45 & 11.49 \\
133408 & 1.45 & 11.49 \\
133409 & 32.80 & 260.08 \\
133410 & 161.15 & 1277.88 \\
133411 & 184.52 & 1463.24 \\
133412 & 178.24 & 1413.42 \\
133413 & 474.59 & 3768.50 \\
133414 & 30.49 & 241.80 \\
133415 & 12.62 & 100.05 \\
133416 & 12.62 & 100.05 \\
133417 & 148.29 & 1175.95 \\
133418 & 161.85 & 1283.49 \\
133419 & 25.34 & 200.95 \\
12230 & 1343.91 & 10657.20 \\
12231 & 208.61 & 1654.25 \\
\end{tabular}
\caption{Cell numbers, volumes and masses of the PPR components of gap 4.}
\end{table}

The F6 tally (or any number ended in 6) calculates the energy deposition in MeV/g-source particle. As neutrons and photons deposit both its energy in the cells, the F6 tally is followed by "N,P", N standing for neutrons and P for photons. In order to calculate the energy deposition, an SD card is used after the F6 tally to input the masses (see Eq. 2.36). It is important to note that when the SD card is used after the F4 tally it inputs volumes (instead of masses), necessary to calculate the particle fluxes across the cells (see Eq. 2.35).

Then a multiplier factor is written in the code in order to output normalised results. Particularly, FM6 will make the F6 tally output power per unit mass in W/g as it follows:

\[
FM6 = \text{Energy deposition} \left( \frac{MeV}{g \text{ source particle}} \right) \times 1.60217662 \times 10^{-13} \left( \frac{J}{MeV} \right) \times \text{Source intensity} \left( \frac{\text{source particle}}{s} \right) = \text{Energy deposition} \times 1.60217662 \times 10^{-13} \times 1.973 \times 10^{19} = 3.1611 \times 10^6 \left( \frac{W}{g} \right).
\]

Where the source intensity is obtained by knowing that 80% of the energy released in ITER is carried by the neutrons and that the MCNP model features only a 40-degree sector of the tokamak (a factor of 40/360 is applied)
Source intensity \( \left( \frac{n}{s} \right) = \frac{0.80 \cdot 500 \ (MW)}{1.60217662 \times 10^{-13} \left( \frac{J}{MeV} \right) \cdot 14.1 \ (MeV) \cdot \frac{40}{360}} \) (3.2)

The following code shows how the nuclear heat loads were calculated:

| F6:N,P | 133401 133402 133403 133404 133405 133406 133407 |
|        | 133408 133409 133410 133411 133412 133413 133414 |
|        | 133415 133416 133417 133418 133419 12230 12231 |
| SD6    | 19.49 19.49 18.51 18.51 17.54 17.54 11.49 11.49 |
|        | 260.08 1277.88 1463.24 1413.42 3763.50 241.80 |
|        | 100.05 100.05 1175.95 1283.49 200.95 |
|        | 10657.20 1654.25 $ masses |
| FM6    | 3.1611E+06 |

Another tally is used to show the neutron contribution and hence the photon contribution to the total nuclear heat load (energy deposition).

| F16:N | 133401 133402 133403 133404 133405 133406 133407 |
|        | 133408 133409 133410 133411 133412 133413 133414 |
|        | 133415 133416 133417 133418 133419 12230 12231 |
| SD16   | 19.49 19.49 18.51 18.51 17.54 17.54 11.49 11.49 |
|        | 260.08 1277.88 1463.24 1413.42 3763.50 241.80 |
|        | 100.05 100.05 1175.95 1283.49 200.95 |
|        | 10657.20 1654.25 $ masses |
| FM16   | 3.1611E+06 |

The F4:N and F14:P tallies calculate the neutron and photon fluxes across the same cells that were input in the F6 tallies. An energy (En) is used to subdivide the flux into energy bins [54].

| F4:N  | 133401 133402 133403 133404 133405 133406 133407 |
|       | 133408 133409 133410 133411 133412 133413 133414 |
|       | 133415 133416 133417 133418 133419 12230 12231 |
| E4    | 1.00E-11 1.00E-10 1.00E-09 1.00E-08 1.00E-07 1.00E-06 |
|       | 2.00E-06 5.00E-06 1.00E-05 2.00E-05 5.00E-05 1.00E-04 |
|       | 2.00E-04 5.00E-04 1.00E-03 2.00E-03 5.00E-03 1.00E-02 |
|       | 2.00E-02 5.00E-02 1.00E-01 2.00E-01 5.00E-01 1.00E+00 |
|       | 1.20E+00 1.40E+00 1.60E+00 1.80E+00 2.00E+00 2.50E+00 |
|       | 3.00E+00 3.50E+00 4.00E+00 4.50E+00 5.00E+00 6.00E+00 |
|       | 7.00E+00 8.00E+00 9.00E+00 1.00E+01 1.10E+01 1.20E+01 |
|       | 1.30E+01 1.40E+01 1.50E+01 1.60E+01 1.71E+01 1.82E+01 |
|       | 1.92E+01 2.00E+01 2.50E+01 3.00E+01 3.50E+01 4.00E+01 |
|       | 4.50E+01 5.00E+01 5.50E+01 6.00E+01 6.50E+01 7.00E+01 |
|       | 7.50E+01 8.00E+01 8.50E+01 9.00E+01 9.50E+01 1.00E+02 |
|       | 1.06E+02 1.10E+02 1.16E+02 1.20E+02 1.26E+02 1.30E+02 |
|       | 1.36E+02 1.40E+02 1.46E+02 1.50E+02 1.54E+02 1.58E+02 |
| SD4   | 2.46 2.46 2.33 2.33 2.21 2.21 1.45 1.45 |
|       | 32.80 161.15 184.52 178.24 474.59 30.49 |
|       | 12.62 12.62 148.29 161.85 25.34 |
|       | 1343.91 208.61 |
Finally, F14:P, E14 and SD14 are written afterwards in the code. The parameters take the same values as F4:N, E4 and SD4.

The power per unit mass from MCNP6 is then multiplied by the density, which is 7.93 g/cm$^3$, in order to obtain the power density or total heat load (W/cm$^3$), which will be used as input to calculate the temperature distribution using ANSYS. The neutron flux spectra obtained in MCNP6 are then used to calculate the DPAs. Figure 30 is a flow chart indicating the basic steps followed.

\[
\text{Power per unit mass (W/g)}
\]
\[
\begin{align*}
\text{F6 tally} \\
\text{SD card} \\
\text{FM (multiplier factor)}
\end{align*}
\]
\[
\text{Power density and temperature distribution using ANSYS.}
\]

\[
\text{Neutron and photon fluence per source particle (particle/cm$^2$source particle)}
\]
\[
\begin{align*}
\text{F4 tally} \\
\text{E4 (energy bins)} \\
\text{SD card}
\end{align*}
\]
\[
\text{DPAs using the treatment of cross sections (NJOY).}
\]

Figure 30: Flow chart showing the followed procedure. Left: MCNP6 outputs using the listed commands in the arrows. Right: Variables obtained.

In order to have meaningful results, the statistical errors of the Monte Carlo simulations were kept below 10%. This value was taken from the guidelines provided in the MCNP manual [43] for interpreting the quality of the simulation results, represented in Table 7.

<table>
<thead>
<tr>
<th>Error</th>
<th>Quality</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5 to 1.0</td>
<td>Not meaningful</td>
</tr>
<tr>
<td>0.2 to 0.5</td>
<td>Factor of a few</td>
</tr>
<tr>
<td>0.1 to 0.2</td>
<td>Questionable</td>
</tr>
<tr>
<td>&lt; 0.10</td>
<td>Generally reliable</td>
</tr>
<tr>
<td>&lt; 0.05</td>
<td>Generally reliable for point detectors</td>
</tr>
</tbody>
</table>

Table 7: Guidelines for interpreting the statistical errors of the simulations [43].

In order to obtain statistical errors below 10%, 1E9 source particles were simulated in each run (nps 1E9).
3.2.3 NJOY PROCEDURE

The NJOY Nuclear Data Processing System is a computer code used for converting evaluated nuclear data in the ENDF format into libraries for several practical applications. ENDF "tapes" are subdivided internally into "materials" (MAT), "files" (MF), and "sections" (MT) [57].

When performing DPA calculations in ITER nuclear analyses the use of the latest version of the Fusion Evaluated Nuclear Data Library (FENDL) is mandatory and it is recommended that natural iron is used as an approximation instead of stainless steel. Cross sections for natural iron were thus applied instead of using the material of the PPR, which is SS316L (N):IG, due to unknown cross sections for some elements such as Sn.

The different isotopes of natural iron in FENDL were identified with the following four numbers (MAT):

- 2625 for Fe54
- 2631 for Fe56
- 2634 for Fe57
- 2637 for Fe58

Once stored as libraries, input files were created according to the following modules:

- **Moder** is the module which converts ENDF “tapes” back and forth between ASCII format and the special NJOY blocked-binary format. Positive unit numbers refer to formatted tapes, and negative unit numbers refer to blocked binary tapes with absolute magnitudes, normally in the range 20-99.

- **Reconr** reconstructs pointwise (energy-dependent) cross sections from ENDF resonance parameters and interpolation schemes. Card 1 in reconr comprises of the first output unit, -21 for the ENDF tape, and the second output unit, -22 assigned for the PENDF tape. Card 2 is the name for the PENDF tape. In this case, it is called ‘material 2625 library’. Then, card 3 indicates the material to be reconstructed (MAT), followed by the number of cards of descriptive data. The criteria used for deciding when to stop halving intervals during resonance reconstruction are complex. Card 4 allows to use the fractional reconstruction tolerance (0.001) and the reconstruction temperature in degree Kelvin (0.). By default, the number of significant figures is 7. Card 5 inputs the descriptive comments for MT451 and card 6 terminates execution of reconr with 0/.

- **Broadr** adds temperature dependence to the pointwise cross sections generated by the reconr module. Card 1 defines the input ENDF tape, the input PENDF tape and the output PENDF tape (23). Card 2 indicates the material to be processed, the number of final temperatures, no restart (0), bootstrap needed as it is faster due to broadening each final temperature from the preceding temperature 1) and starting temperature (0 Kelvin). Card 3 is the fractional tolerance for thinning. Card 4 is the final temperature in degree Kelvin and card 5 terminates execution of broadr with 0/.

- **Heatr** can be used to compute estimates of energy-deposition cross sections for neutrons that can be combined with calculations of neutron fluxes in nuclear systems to compute the
neutronics contributions to nuclear heating. Recoil nuclei from scattering reactions and energetic charged particles being slowed down by nuclear reactions that lead to heating can also cause damage to the crystalline structure of the materials that they pass through. *Heatr* computes the damage-production energy, which can be correlated to macroscopic damage through phenomenological factors like DPA. Card 1 uses the unit ENDF tape, the unit for the input PENDF tape (23, which is the output of the *broadr* module) and the unit for the output PENDF (33). Card 2 indicates the material to be processed, the number of partial kermas desired (1), the number of user q-values and temperatures to process (0) and just check the command iprint (2). Card 3 asks for the type of damage energy production: 444 is the total damage energy production.

- The *Gaspr* module goes through all of the reactions given in an ENDF-format evaluation, determines which charged particles (proton, deuteron, triton, He-3 or alpha) would be produced by the reaction, and adds up the particle yield times the reaction cross section to produce the desired gas production cross sections. It uses data from an input ENDF tape and an input PENDF tape (33 from the output *heatr* module), and it writes the results on an output PENDF tape, 34.

- *Unresr* calculates effective self-shielded pointwise cross sections in the unresolved energy range. Card 1 specifies the input and output units for the module. Card 2 specifies the material desired (MAT), the number of temperatures and background cross sections and the print option. Card 3 is used to specify the temperature in Kelvin. Card 4 inputs the sigma zero values and card 5 terminates execution of *unresr*.

- *Groupr* generates multigroup cross sections. In order to obtain several "responses," such as heating, production of a radionuclide, or production of helium, it is common to reduce the detail in the pointwise cross sections by averaging them over a set of energy ranges called "groups." The *groupr* module of *NJOY* also generates multigroup "matrices," which describe the transfer of neutrons from one group to another. It is written in card 1 the unit for ENDF tape, the unit for PENDF tape and the input (default=0) and output GOUT tape (a GENDF file, which is a multigroup version of an ENDF tape). Card 2 specifies the material to be processed (MAT), the neutron group structure option, then the gamma group structure option, the weight function, the Legendre order, the number of temperatures, the number of sigma zeroes and the print option for minimum. Card 3 then gives a title to library. Card 4 is the temperature in Kelvin. Card 5 is the sigma zero values. Card6a is the number of groups and card 6b is the group breaks.

For the material Fe-54, the code for the input data was the following:

```
moder
20 -21
reconr
-21 -22
'material 2625 library'/
2625 1/
.001 0. 7/
'material 2625 library'/
```
<table>
<thead>
<tr>
<th>Material</th>
<th>Symbol</th>
<th>Density (g/cm³)</th>
<th>Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>broadr</td>
<td>-21-22-23</td>
<td>2625 1 0 1 0</td>
<td>0.001</td>
</tr>
<tr>
<td>heatr</td>
<td>-21-23-33</td>
<td>2625 1 0 0 0 2</td>
<td>444</td>
</tr>
<tr>
<td>gaspr</td>
<td>-21-33-34</td>
<td>2625 1 1 0</td>
<td>300</td>
</tr>
<tr>
<td>unresr</td>
<td>-21-34-24</td>
<td>2625 1 1 0</td>
<td>300</td>
</tr>
<tr>
<td>groupr</td>
<td>-21-24 0 27</td>
<td>'material 2625 library'</td>
<td>300</td>
</tr>
</tbody>
</table>

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1.000E-05 1.000E-01 4.140E-01 5.316E-01 6.826E-01 8.764E-01 1.125E+00
1.445E+00 1.855E+00 2.382E+00 3.059E+00 3.928E+00 5.043E+00 6.476E+00
8.315E+00 1.068E+00 1.371E+00 1.760E+00 2.260E+00 2.902E+00 3.727E+00
4.785E+01 6.144E+01 7.889E+01 1.013E+02 1.301E+02 1.670E+02 2.144E+02
2.754E+02 3.536E+02 4.540E+02 5.830E+02 7.485E+02 9.611E+02 1.234E+03
1.585E+03 2.035E+03 2.249E+03 2.485E+03 2.613E+03 2.746E+03 3.035E+03
3.355E+03 3.707E+03 4.307E+03 5.531E+03 7.102E+03 9.119E+03 1.060E+04
1.171E+04 1.503E+04 1.930E+04 2.188E+04 2.358E+04 2.418E+04 2.479E+04
2.606E+04 2.700E+04 2.850E+04 3.183E+04 3.431E+04 4.087E+04 4.631E+04
9.804E+04 1.111E+05 1.168E+05 1.228E+05 1.291E+05 1.357E+05 1.426E+05
1.500E+05 1.576E+05 1.657E+05 1.742E+05 1.832E+05 1.926E+05 2.024E+05
2.128E+05 2.237E+05 2.352E+05 2.472E+05 2.732E+05 2.872E+05 2.945E+05
2.972E+05 2.985E+05 3.020E+05 3.337E+05 3.688E+05 3.877E+05 4.076E+05
4.505E+05 4.979E+05 5.234E+05 5.502E+05 5.784E+05 6.081E+05 6.393E+05
6.721E+05 7.065E+05 7.427E+05 7.808E+05 8.208E+05 8.629E+05 9.072E+05
9.616E+05 1.003E+06 1.108E+06 1.165E+06 1.225E+06 1.287E+06 1.353E+06
1.423E+06 1.496E+06 1.572E+06 1.653E+06 1.738E+06 1.827E+06 1.920E+06
2.019E+06 2.122E+06 2.231E+06 2.307E+06 2.346E+06 2.365E+06 2.385E+06
2.466E+06 2.592E+06 2.725E+06 2.865E+06 3.012E+06 3.166E+06 3.329E+06
3.679E+06 4.066E+06 4.493E+06 4.724E+06 4.966E+06 5.220E+06 5.488E+06
5.770E+06 6.065E+06 6.376E+06 6.592E+06 6.703E+06 7.047E+06 7.408E+06
7.788E+06 8.187E+06 8.607E+06 9.048E+06 9.512E+06 1.000E+07 1.051E+07
1.105E+07 1.162E+07 1.221E+07 1.252E+07 1.284E+07 1.350E+07 1.384E+07
1.419E+07 1.455E+07 1.492E+07 1.568E+07 1.649E+07 1.690E+07 1.733E+07
1.964E+07 2.000E+07 2.100E+07 2.200E+07 2.300E+07 2.400E+07 2.500E+07
2.600E+07 2.700E+07 2.800E+07 2.900E+07 3.000E+07 3.100E+07 3.200E+07
2.600E+07 2.700E+07 2.800E+07 2.900E+07 3.000E+07 3.100E+07 3.200E+07

Card 2 was modified in each module with the material number desired and the rest of the code was kept constant for the remaining materials. NJOY was run after creating the following batch files for every single material:

```
echo NJOY, DPA Fe54
echo getting endf tape for Fe-54
copy ..\2625Fe54 tape20
pause
echo running njoy
..\njoy<inFe54.dat
pause
echo saving output file
copy output out13
```

### 3.2.4 Displacement Per Atom (DPA)

A widely-used measure of radiation damage, displacement per atom (DPA) is a quantity used to assess the irradiation effect on the thermomechanical properties of the materials. If more energy incomes to an atom by nuclear bombardment than the displacement energy, the atom will leave its equilibrium position in the lattice, leaving behind a vacancy (Frenkel pair). This atom is known as the Primary Knock-on Atom (PKA) and can subsequently induce displacements of other atoms in the lattice if it possesses sufficient energy, or come to rest in the lattice at an interstitial site if it does not \[58][59].

DPAs can be calculated using Eq. 3.2 [60]:

$$DPA = \left( \int \sigma_{DX}(E) \cdot \phi(E) \cdot dE \right) t,$$

where $\sigma_{DX}(E)$ is the displacement cross section for an incident particle at an energy $E$, $\phi(E)$ the incident particle flux or neutrons obtained from MCNP6 and $t$ is the irradiation time. In general, $\sigma_{DX}(E)$ can be obtained from the following expression:

$$\sigma_{DX}(E) = \sum_{i} \int_{T_d}^{T_{max}} v_d(T) \cdot \frac{d\sigma_{DX}^{i}(T,E)}{dT} \cdot dT,$$

where $T$ is the PKA energy, $T_d$ is the atomic threshold displacement energy, $T_{max}$ the maximum of $T$, $v_d(T)$ the displacement damage function and $\frac{d\sigma_{DX}^{i}(T,E)}{dT}$ is the energy-differential cross section for the $i$-th element. The values of $\frac{d\sigma_{DX}^{i}(T,E)}{dT}$ are calculated by NJOY with the evaluated library. $v_d(T)$ is expressed by
The following equation proposed by Norgett, Torrens and Robinson, based on the earlier Kinchin-Pease model [61].

\[ \nu_d(T) = \frac{\beta}{2T_d} \cdot T_d \text{a}, \]

where \( \beta \) is the constant 0.8 [61], \( T_d \text{a} \) the damage energy and the \( T_d \) values are listed in Table 8 [62]:

<table>
<thead>
<tr>
<th>Material</th>
<th>Atomic displacement energy in NJOY, Td (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be</td>
<td>31</td>
</tr>
<tr>
<td>C</td>
<td>31</td>
</tr>
<tr>
<td>Al</td>
<td>27</td>
</tr>
<tr>
<td>Cr</td>
<td>40</td>
</tr>
<tr>
<td>Fe</td>
<td>40</td>
</tr>
<tr>
<td>Ni</td>
<td>40</td>
</tr>
<tr>
<td>Cu</td>
<td>40</td>
</tr>
<tr>
<td>Pb</td>
<td>25</td>
</tr>
</tbody>
</table>

Table 8: Atomic displacement energy \( T_d \) in NJOY (eV) for some materials.

The method used to obtain the DPAs is summarized in Figure 31.

![Flow chart showing the variables needed for calculating the DPAs.](image)

Figure 31: Flow chart showing the variables needed for calculating the DPAs.

DPAs can be calculated per lifetime and per year at full power capacity. Note that the F4 tally from MCNP6 was left without normalisation as the source strength is not constant during the lifetime of ITER. Table 9 shows the irradiation profile foreseen for ITER.

For each cell, a spreadsheet was created with the following columns:

- Energy bins (MeV).
- Tally F4 from MCNP6: Fluence per source particle.
- Fluxes (neutrons and gamma/cm²s) obtained by multiplying fluence and source strengths. (Five columns for every source strength).
- NJOY cross sections in barns for every iron element (2625, 2631, 2634, 2637).
Then for each i-isotope the DPAs per year were calculated for every source strength j:

$$DPA^{i,j} \text{ (year}^{-1}) = \frac{\varphi(\text{or gamma/cm}^2\text{s}) \cdot \sigma(\text{barns}) \cdot 1 \times 10^{-24} \text{cm}^2\text{barn} \cdot 0.8 \cdot 3600 \left(\frac{s}{h}\right) \times 24 \left(\frac{h}{day}\right) \times 365 \left(\frac{day}{year}\right)}{Td \ (eV)}$$

(3.6)

DPAs in ITER's lifetime for each isotope are calculated afterwards:

$$DPA^i \ (\text{lifetime}) = \sum_{j=1}^{5} DPA^j \ (\text{per year}) \times \text{years},$$

(3.7)

Finally, the overall effect on the different N isotopes is taken into account and integration is done over the energy spectrum [63]:

$$DPA = \frac{\int dE \varphi(\vec{r}, E) \sum_{i=1}^{N} \rho_i \sigma_{R,\text{DPA},i}(E)}{\sum_{i=1}^{N} \rho_i},$$

(3.8)

in which $\varphi(\vec{r}, E)$ is the neutron flux (cm$^{-2}$s$^{-1}$MeV$^{-1}$), $\rho_i$ is the atom density (barn$^{-1}$cm$^{-1}$) for isotope i and $\sigma_{R,\text{DPA},i}$ is the DPA cross section (barns/atom) for isotope i at energy E.
4 RESULTS

4.1 Shielding sphere

A geometry was implemented to see the effect of ionizing radiation and to serve as a model for the MMA interface. Neutrons may interact with matter through elastic collisions, whereby energy is loss. Depending on the atomic mass of the target nucleus, the average number of collisions required to thermalize the neutrons is different. As Table 3 shows, the greater the atomic mass the higher the average number of collisions needed.

Figure 32 shows the mesh tally obtained from MCNP6 for the lead-shielded sphere. The neutron flux in lead is higher than the one estimated for the water-shielded sphere (See Figure 33). This shows that water is indeed a better neutron moderator than lead, as discussed in section 2.2.1.

![Neutron flux (n/cm²s) across the lead shielding cells.](image-url)
Figure 33: Neutron flux (n/cm²s) across the water shielding cells.

Figure 34: Photon flux (Ɣ/cm²s) across the lead shielding cells.
According to the results in Figure 34 and Figure 35, there are lower photon fluxes in water than in lead. Contrary to what happens with neutrons, this does not mean that water is a better shielding material for photons than lead, which is not the case; it is rather due to the fact that in water the photons are produced in the inner layers.

Figure 35: Photon flux (\(\gamma/cm^2s\)) across the water shielding cells.

More layers were added to improve the resolution of the results in the inner cells, following the methodology described in section 3.1.1. The resulting geometry configuration is shown in Figure 36.
Figure 36: New geometry implemented.

Figure 37 shows the neutron flux spectra in each of the surfaces of the lead shielding. It can be seen that as we get further away from the neutron source, the neutron and the photon fluxes are reduced at all energies, as absorption of particles takes place.

Figure 37: Neutron flux across the lead shielding surfaces.
When the 14-MeV neutrons released by the source interact with the shielding material, inelastic scattering and radiative capture occur, resulting in the emission of photons with particular energies in order to bring the nucleus back down to a stable or ground state. This explains the several peaks in the photon flux spectra, at 11.6 keV, 82.5 keV, 53.1 keV and 7.5 MeV, as shown in Figure 38.

The neutron fluxes in water (see Figure 39) follow an irregular distribution but the spectra are softer than in lead (Figure 37).

In water, Figure 40 shows that there are also peaks in the photon fluxes but they are concentrated in the region from 2 to 10 MeV.
Figure 40: Photon fluxes across the water shielding surfaces.

The comparison between water and lead for surface 6 (75 cm of width) can be seen in Figure 41. The higher neutron fluxes at higher energies in water are due to the fact that water has a much lower density than lead, and therefore more un-collided neutrons reach surface 6 with water than with lead. For lower energies, the fluxes are more similar. The exception is for energies between 0.025 eV and 10 eV, where the fluxes are higher for water by more than one order of magnitude, which shows that water is more effective at thermalizing neutrons.

Figure 41: Neutron and photon fluxes across the lead and water shielding surface 6.
Figure 42 shows the heat loads in each cell for the two shielding materials. For water, more energy is deposited in the first cell (cell number 2), whereas more energy is deposited in lead from cell 3 onwards.

Figure 42: Power density in each cell for the lead and water shielding layers.

Figure 43: Steady-state thermal analysis for lead shielding.
The temperature distribution is shown in Figure 43 and Figure 44. Results show that both materials are not suitable for the source intensity of $2 \times 10^{19}$ source particles/s. The maximum temperature reached with lead is 817.24 °C, above the melting point of 327.5 °C. Only the outer layers can withstand the temperature. This happens because water has a very low conductivity when compared to lead, yielding extremely high temperatures (of the order of $2.6 \times 10^5$ °C).

![Steady-state thermal analysis](image)

Figure 44: Steady-state thermal analysis for water shielding.

4.2 PPR system

4.2.1 POWER DENSITY

According to the methodology described in section 3.2.2 (MCNP procedure), the power density was calculated for each cell, which is the total power density that the structure needs to withstand. The estimated power density in the PPR in-vessel components due to ionizing radiation are presented in Table 10. Relative contributions of neutrons and gamma photons to the energy deposition in each cell are also achieved by simulation in MCNP6.

The most exposed parts to irradiation are the tips of the antennas, where the heat loads are predicted to be of the order of 3.8 W/cm$^3$, decreasing steadily up to cell 133414, which is already located behind
BM#11. There is an increase in energy deposition in cells 133415 and 133416 (located side-by-side) due to an increase in heat load by photons while maintaining approximately the same heat load induced by neutrons in cells 133414, 133415 and 133416. The power density for cells 133417, 133418, 133419 and 12231 are lower, implying thus that the opening between the blanket module and the upper port has little effect on the power density in these cells.

<table>
<thead>
<tr>
<th>Cell</th>
<th>Total power density (W/cm²)</th>
<th>Stat. Error (%)</th>
<th>Power density by Neutrons (W/cm²)</th>
<th>Stat. Error (%)</th>
<th>Power density by Neutrons (%)</th>
<th>Power density by Photons (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>133401</td>
<td>3.7361</td>
<td>1.92</td>
<td>0.5857</td>
<td>2.76</td>
<td>15.7</td>
<td>84.3</td>
</tr>
<tr>
<td>133402</td>
<td>3.7779</td>
<td>1.90</td>
<td>0.6028</td>
<td>2.78</td>
<td>16.0</td>
<td>84.0</td>
</tr>
<tr>
<td>133403</td>
<td>3.0941</td>
<td>2.21</td>
<td>0.4836</td>
<td>3.33</td>
<td>15.6</td>
<td>84.4</td>
</tr>
<tr>
<td>133404</td>
<td>3.0397</td>
<td>2.08</td>
<td>0.4687</td>
<td>3.12</td>
<td>15.4</td>
<td>84.6</td>
</tr>
<tr>
<td>133405</td>
<td>2.2791</td>
<td>2.45</td>
<td>0.4016</td>
<td>3.75</td>
<td>17.6</td>
<td>82.4</td>
</tr>
<tr>
<td>133406</td>
<td>2.9219</td>
<td>2.42</td>
<td>0.3668</td>
<td>3.68</td>
<td>12.6</td>
<td>87.4</td>
</tr>
<tr>
<td>133407</td>
<td>1.9908</td>
<td>3.43</td>
<td>0.3155</td>
<td>4.79</td>
<td>15.8</td>
<td>84.2</td>
</tr>
<tr>
<td>133408</td>
<td>1.9227</td>
<td>3.24</td>
<td>0.3091</td>
<td>5.00</td>
<td>16.1</td>
<td>83.9</td>
</tr>
<tr>
<td>133409</td>
<td>1.5103</td>
<td>1.67</td>
<td>0.2218</td>
<td>2.20</td>
<td>14.7</td>
<td>85.3</td>
</tr>
<tr>
<td>133410</td>
<td>0.8384</td>
<td>1.45</td>
<td>0.0995</td>
<td>1.89</td>
<td>11.9</td>
<td>88.1</td>
</tr>
<tr>
<td>133411</td>
<td>0.4726</td>
<td>1.84</td>
<td>0.0440</td>
<td>2.43</td>
<td>9.31</td>
<td>90.7</td>
</tr>
<tr>
<td>133412</td>
<td>0.2790</td>
<td>2.21</td>
<td>0.0237</td>
<td>2.89</td>
<td>8.49</td>
<td>91.5</td>
</tr>
<tr>
<td>133413</td>
<td>0.1698</td>
<td>2.20</td>
<td>0.0124</td>
<td>2.75</td>
<td>7.30</td>
<td>92.7</td>
</tr>
<tr>
<td>133414</td>
<td>0.1070</td>
<td>6.40</td>
<td>0.0049</td>
<td>7.27</td>
<td>4.58</td>
<td>95.5</td>
</tr>
<tr>
<td>133415</td>
<td>0.1342</td>
<td>4.77</td>
<td>0.0057</td>
<td>7.30</td>
<td>4.25</td>
<td>95.8</td>
</tr>
<tr>
<td>133416</td>
<td>0.1364</td>
<td>4.64</td>
<td>0.0048</td>
<td>6.08</td>
<td>3.52</td>
<td>96.5</td>
</tr>
<tr>
<td>133417</td>
<td>0.0831</td>
<td>4.14</td>
<td>0.0033</td>
<td>4.76</td>
<td>3.97</td>
<td>96.0</td>
</tr>
<tr>
<td>133418</td>
<td>0.0658</td>
<td>4.40</td>
<td>0.0031</td>
<td>6.45</td>
<td>4.71</td>
<td>95.2</td>
</tr>
<tr>
<td>133419</td>
<td>0.0753</td>
<td>8.70</td>
<td>0.0037</td>
<td>11.8</td>
<td>4.91</td>
<td>95.1</td>
</tr>
<tr>
<td>12230</td>
<td>0.0072</td>
<td>6.36</td>
<td>0.0004</td>
<td>9.08</td>
<td>5.56</td>
<td>94.4</td>
</tr>
<tr>
<td>12231</td>
<td>0.0868</td>
<td>3.60</td>
<td>0.0044</td>
<td>4.85</td>
<td>5.07</td>
<td>94.9</td>
</tr>
</tbody>
</table>

Table 10: Power density in the PPR components of gap 4.

It is clear that photons contribute the most, from approximately 84% to 96.5% of the total heat load. This is due to the fact that PPR components are made of stainless steel, a High-Z material and therefore more effective to shield photons than neutrons (see Section 4.1). The statistical errors of all tallies are below 10% except for cell 133419. This is due to the large amount of CPU time that is required in order to perform the simulations with such a complex geometry. The results of cell 133419 are, however, consistent with the results obtained for the neighbouring cells.

4.2.2 Temperature distribution

The results in the PPR system for the temperature were obtained in a previous work [64], following the methodology described in section 3.3.1, and are included here to complement the analysis. The 20-
node thermal FEs were chosen with a single degree-of-freedom at each node (temperature). The following boundary conditions were used:

- An environment temperature of 150°C.
- A radiation power per unit area of 500 kW/m².

At first, it is considered that the system will reach the steady-state regime in order to prove the consistency of the model.

Furthermore, it is assumed that the material is a grey body, the absorptivity is equal to the emissivity, which, like other properties, is dependent on the temperature. Two emissivity conditions were applied:

a. the exterior and inner surfaces of the antenna have equal emissivity values.

b. the exterior surface of the antenna has an emissivity value similar to that of the blanket modules surfaces, whereas the inner surfaces of the antenna keep the initial emissivity values.

Figure 45: Steady-state temperature distribution of the PPR in-vessel components [64].

Figure 45 illustrates that the maximum temperature achieved is at the tips of the antennas: approximately 759°C for emissivity condition a) and 714°C for emissivity condition b). [64]. Hence, emissivity condition b) is recommended for lower temperature operation.
As for the transient temperature analysis, it is considered that ITER will operate in 400-second cycles and with an initial temperature of 150°C. Figure 46 shows that steady-state conditions are not achieved; temperatures are lower than the ones obtained in Figure 45. For emissivity condition a), the tips of the antennas reach a maximum temperature of approximately 713°C. For emissivity condition b), the tips of the antennas reach a maximum temperature of approximately 702°C [64]. Thus, emissivity condition b) is again recommended, although the tips of the antennas present lower maximum temperatures before t=350 s.

4.2.3 DPAs

According to the methodology described in sections 3.2.2 and 3.2.4, the energy cross sections were obtained from NJOY and the library FENDL 3.1. Figure 47 shows the output from NJOY compared to the latest set of cross sections available in the JANIS program (FENDL2.1). The comparison illustrates how NJOY changes from pointwise cross sections to energy groups.

The material chosen as an approximation for stainless steel 316L (N)-IG is natural iron, for which the value of Td is 40 eV. For every single isotope, DPAs are calculated over all the spectrum, slightly overestimating results as there is a low boundary of 40 eV that is not considered. Figure 48 shows the cross sections obtained from NJOY in barns for the four isotopes of natural iron. DPAs are summed up according to their weight composition: Fe-54 is 5.845%, Fe-56 is 91.754%, Fe-57 is 2.119% and 0.282% of the composition of natural iron is Fe-58.
The DPA results are summarized in Table 12. DPAs reach a maximum value of 1.2 during the lifetime of ITER at the antenna tips for being exposed to higher levels of neutron fluxes for cells 133401 and 133402. Note that the DPA calculated is approximately the same for cell 133401, as they are adjacent cells and exposed to the approximately the same neutron fluence. In general terms, DPAs are decreasing at a steady rate as the neutron fluence decreases as shown in Figure 49 and
Table 11: Neutron fluence, neutron flux at full power and total statistical error from MCNP6.

<table>
<thead>
<tr>
<th>Cell number</th>
<th>Neutron fluence (n/cm² source particle)</th>
<th>Neutron flux at full power (n/cm²s)</th>
<th>Total statistical error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>133401</td>
<td>4.89E-06</td>
<td>9.78E+13</td>
<td>1.13</td>
</tr>
<tr>
<td>133402</td>
<td>4.90E-06</td>
<td>9.80E+13</td>
<td>1.12</td>
</tr>
<tr>
<td>133403</td>
<td>4.32E-06</td>
<td>8.65E+13</td>
<td>1.26</td>
</tr>
<tr>
<td>133404</td>
<td>4.26E-06</td>
<td>8.53E+13</td>
<td>1.23</td>
</tr>
<tr>
<td>133405</td>
<td>3.69E-06</td>
<td>7.37E+13</td>
<td>1.39</td>
</tr>
<tr>
<td>133406</td>
<td>3.67E-06</td>
<td>7.34E+13</td>
<td>1.38</td>
</tr>
<tr>
<td>133407</td>
<td>3.20E-06</td>
<td>6.40E+13</td>
<td>1.75</td>
</tr>
<tr>
<td>133408</td>
<td>3.15E-06</td>
<td>6.30E+13</td>
<td>1.75</td>
</tr>
<tr>
<td>133409</td>
<td>2.70E-06</td>
<td>5.39E+13</td>
<td>0.91</td>
</tr>
<tr>
<td>133410</td>
<td>1.84E-06</td>
<td>3.68E+13</td>
<td>0.83</td>
</tr>
<tr>
<td>133411</td>
<td>1.20E-06</td>
<td>2.41E+13</td>
<td>0.95</td>
</tr>
<tr>
<td>133412</td>
<td>8.20E-07</td>
<td>1.64E+13</td>
<td>1.05</td>
</tr>
<tr>
<td>133413</td>
<td>5.60E-07</td>
<td>1.12E+13</td>
<td>1.08</td>
</tr>
<tr>
<td>133414</td>
<td>3.60E-07</td>
<td>7.20E+12</td>
<td>2.35</td>
</tr>
<tr>
<td>133415</td>
<td>3.14E-07</td>
<td>6.28E+12</td>
<td>2.13</td>
</tr>
<tr>
<td>133416</td>
<td>3.30E-07</td>
<td>6.59E+12</td>
<td>1.98</td>
</tr>
<tr>
<td>133417</td>
<td>2.55E-07</td>
<td>5.10E+12</td>
<td>1.81</td>
</tr>
<tr>
<td>133418</td>
<td>2.48E-07</td>
<td>4.96E+12</td>
<td>1.75</td>
</tr>
<tr>
<td>133419</td>
<td>2.59E-07</td>
<td>5.19E+12</td>
<td>3.01</td>
</tr>
<tr>
<td>12230</td>
<td>2.41E-08</td>
<td>4.83E+11</td>
<td>2.11</td>
</tr>
<tr>
<td>12231</td>
<td>3.27E-07</td>
<td>6.54E+12</td>
<td>1.30</td>
</tr>
</tbody>
</table>

Figure 49: Neutron fluence for the two cells selected.
The DPAs calculated at full power capacity with an intensity of $2 \times 10^{19}$ particles/s are less than double the DPAs reached in ITER's lifetime. This is due to the short period under which the PPR in-vessel components are exposed to full power capacity: 17 cycles of 400 seconds exposure combined with 3920 seconds without irradiation.

In addition, DPAs are within the expected values for a fusion reactor: according to reference [65], the maximum value expected for ITER in the blanket is 3 DPA.

<table>
<thead>
<tr>
<th>Cell number</th>
<th>DPA (in ITER's lifetime)</th>
<th>DPA (per year 500MW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>133401</td>
<td>1.19E+00</td>
<td>2.22E+00</td>
</tr>
<tr>
<td>133402</td>
<td>1.20E+00</td>
<td>2.25E+00</td>
</tr>
<tr>
<td>133403</td>
<td>9.89E-01</td>
<td>1.85E+00</td>
</tr>
<tr>
<td>133404</td>
<td>9.71E-01</td>
<td>1.82E+00</td>
</tr>
<tr>
<td>133405</td>
<td>8.34E-01</td>
<td>1.56E+00</td>
</tr>
<tr>
<td>133406</td>
<td>7.86E-01</td>
<td>1.47E+00</td>
</tr>
<tr>
<td>133407</td>
<td>6.70E-01</td>
<td>1.25E+00</td>
</tr>
<tr>
<td>133408</td>
<td>6.66E-01</td>
<td>1.25E+00</td>
</tr>
<tr>
<td>133409</td>
<td>5.01E-01</td>
<td>9.38E-01</td>
</tr>
<tr>
<td>133410</td>
<td>2.60E-01</td>
<td>4.86E-01</td>
</tr>
<tr>
<td>133411</td>
<td>1.33E-01</td>
<td>2.49E-01</td>
</tr>
<tr>
<td>133412</td>
<td>7.74E-02</td>
<td>1.45E-01</td>
</tr>
<tr>
<td>133413</td>
<td>4.63E-02</td>
<td>8.67E-02</td>
</tr>
<tr>
<td>133414</td>
<td>2.25E-02</td>
<td>4.21E-02</td>
</tr>
<tr>
<td>133415</td>
<td>2.10E-02</td>
<td>3.93E-02</td>
</tr>
<tr>
<td>133416</td>
<td>2.05E-02</td>
<td>3.84E-02</td>
</tr>
<tr>
<td>133417</td>
<td>1.53E-02</td>
<td>2.87E-02</td>
</tr>
<tr>
<td>133418</td>
<td>1.47E-02</td>
<td>2.75E-02</td>
</tr>
<tr>
<td>133419</td>
<td>1.73E-02</td>
<td>3.24E-02</td>
</tr>
<tr>
<td>12230</td>
<td>1.67E-03</td>
<td>3.13E-03</td>
</tr>
<tr>
<td>12231</td>
<td>2.16E-02</td>
<td>4.04E-02</td>
</tr>
</tbody>
</table>

Table 12: DPAs per lifetime and per year at full power capacity for every cell.

Results are also complemented with FISPACT [66] calculations performed in the group, which are provided in Table 13 to show the production of H and He in one of the cells exposed to higher radiation levels (133401). It can be seen that the production of He in stainless steel (32 appm) is below the maximum value of 75 appm predicted in reference [65]. As there are many more elements in stainless steel than in iron, the appm values for H and He are much higher in the former.
Table 13: Atomic parts per million of helium and hydrogen produced in iron and stainless steel, for cell 133401.

<table>
<thead>
<tr>
<th>Element</th>
<th>Appm for iron</th>
<th>Appm for stainless steel</th>
</tr>
</thead>
<tbody>
<tr>
<td>He 4</td>
<td>2.0995E+01</td>
<td>3.2301E+01</td>
</tr>
<tr>
<td>He 3</td>
<td>4.9213E-05</td>
<td>1.2709E-03</td>
</tr>
<tr>
<td>H 3</td>
<td>1.5839E-03</td>
<td>5.3139E-02</td>
</tr>
<tr>
<td>H 2</td>
<td>2.0844E+00</td>
<td>2.5052E+00</td>
</tr>
<tr>
<td>H 1</td>
<td>1.1426E+02</td>
<td>1.5632E+02</td>
</tr>
</tbody>
</table>

Associated radiation effects include an increase in swelling for the high operating temperatures in ITER [65] and irradiation hardening, as well as the reduction of fracture toughness and ductility by more than 5.5% [67].

As stated in [68 p.27], “the aim of level A criteria for ITER is to protect the component against the following damage: immediate plastic collapse, immediate plastic instability, immediate plastic flow localization, fast fracture, local fracture due to exhaustion of ductility, ratcheting, fatigue, thermal creep and buckling. The satisfaction of level A criteria is intended to ensure the safety with regard to these types of damage for the specified operation throughout the life of the component.”

Furthermore, according to [69 p.65], “the maximum allowable temperature for 316L (N)-IG stainless steel shall not exceed 600°C without irradiation and up to 450°C for irradiations up to 10 dpa for the criteria Level A”.

Since the predicted DPA values are below 10, the maximum allowable temperature of operation for SS316L(N)-IG to meet the ITER Level A criteria is therefore 450°C. As current estimations predict that the system will reach temperatures as high as 702°C (see Figure 45), the current configuration does not comply with ITER requirements. This means that alternative configurations and materials must be tested, at least for the antennas, where the highest temperatures are reached.

The DPA values calculated in this work complement the results presented in the “Report on the Nuclear Analysis of the In- vessel Components of gap 4” [11], allowing for a complete understanding of the operation conditions of the PPR system from the neutronics point of view. Complemented with the thermal analyses, it is now possible to identify the weaknesses of the current configuration and to establish an important milestone to be achieved: optimize the system so that it is able to operate below 450°C.
5 **CONCLUSION AND FUTURE WORK**

As a first step in this work, a shielding sphere was implemented in order to learn the basics regarding the interaction of neutrons and photons with matter and how the nuclear energy deposition in the materials is translated from MCNP to ANSYS in order to obtain the operation temperatures. Results show that High-Z materials are appropriate for stopping photons, whereas Low-Z materials are suitable for neutron shielding, as expected. An example is lead, which is used as a shielding material for photons, and water, which is mainly used in nuclear power plants to moderate neutrons. When analysing photons through the mesh tally, there is a higher flux in lead due to the increase in production of photons in the outer cells. Finally, the temperature distribution is analysed, showing that both materials (especially water) will reach high temperatures when exposed to a source of neutrons with an intensity comparable to the one foreseen for ITER.

In addition, the interface MMA allows for an automatic translation between MCNP and ANSYS with the capability of changing the following parameters: conductivity and density of the material, atomic number of the element used as shielding material, source intensity and ambient temperature. The automatized procedure allows the user to save time when calculating the temperature distribution on the sphere under different operation conditions.

According to the results obtained in the PPR, the power density is greater at the tips of the antennas, as they are exposed to higher levels of neutron and photon fluxes. Furthermore, emissivity condition b), where the outer surfaces of the PPR components have the same value of the emissivity of the blanket module, is recommended as a solution to decrease the temperature. However, 702°C still exceeds the maximum allowable temperature of 450°C for irradiations up to 10 DPA, necessary to comply with the ITER requirements. Nevertheless, the DPA values are within the expected margins (1.2 DPA per lifetime) and may be used to analyse effects such as swelling and reduction in ductility.

An optimization study showed that by increasing the thickness of the antennas, a temperature decrease of approximately 100°C can be achieved. Another possible solution is the shift of the position of the PPR backwards in order to decrease neutron and photon irradiation, which, however, may compromise the performance of the system. The change of material is another possibility, tungsten being a potential candidate, due to its high melting point and resistance to irradiation.

Hopefully, I will continue this work during my Ph.D. and be able to perform a complete neutronics and mechanical analysis, as well as extend the development of the MMA interface for different configurations.
BIBLIOGRAPHY


ANNEX I: MCNP6 CODE FOR SHIELDING SPHERE

(SHIELDINGSHERE.TXT)

C Cell cards
1 0 -1 $source
2 1 -1 1 -2 $8 water shielding layers
3 1 -1 2 -3
4 1 -1 3 -4
5 1 -1 4 -5
6 1 -1 5 -6
7 1 -1 6 -7
8 1 -1 7 -8
9 1 -1 8 -9
10 1 -1 9 -10
11 2 -1 -11 $water sphere
12 0 11 10 $cell around the water sphere
13 0 12 $outer space

C Surface cards
1 So 400 $sphere source radius R=4 m
2 So 420 $shielding layers
3 So 440
4 So 460
5 So 480
6 So 500
7 So 600
8 So 700
9 So 800
10 So 900
11 SZ 910 10
12 So 1000

C Data cards
mode n p
PRINT
IMP:N,P 1 1 1 1 1 1 1 1 1 1 1 1 0
SDEF pos=0 0 0 rad=d1 cel=1 erg=14 par=N
SI1 0 400 $ radial sampling range: 0 to Rmax
SP1 -21 2 $ weighting for radial sampling: here r^2
F2:N 2 3 4 5 6 7 8 9 10 $average neutron fluxes across each shielding surface
E2 1e-5 100log 20 $from 10 eV to 20 MeV takes log spacing
F12:P 2 3 4 5 6 7 8 9 10
E12 1e-3 100log 20
F4:N 11 $neutron flux across the water sphere cell
E4 1e-5 100log 20
F14:P 11
E14 1e-3 100log 20 $Energy photons!
F6:N,P 2 3 4 5 6 7 8 9 10 $energy deposition across each shielding cell
NPS 100000
c tmesh
c rmesh31:n FLUX
c cora31 -1000 99i 1000
c corb31 -400 4i 400
c corc31 -1000 99i 1000
c endmd
c fm31 1.97e19
M2 1001 2 8016 1 $Water
fm4 1.97e19
ANNEX II: ANSYS APDL (SHIELDINGSphere.inp)

RUN_BATCH=1  !* 0 for manually  and  1 for batch
!*====================================================================
/PREP7

*IF,RUN_BATCH,EQ,0,then

FINISH
/CLEAR,START
/COM,ANSYS RELEASE Release 17.1 BUILD 17.1 UP20160404 02:39:39
/input,start.ans,'C:\Program Files\ANSYS Inc\v171\ANSYS\apdl\'
!* /PREP7

KXXa=35.3  !Conductivity
DENSa=11340  !Density
HGEN1=422035  !Heat generation
HGEN2=117225
HGEN3=7.46743000000000e+04
HGEN4=1.84432000000000e+04
HGEN5=1.08416000000000e+04
HGEN6=9.23094000000000e+03
HGEN7=0.00290205000000
HGEN8=0
HGEN9=0
Tempout=298.15  !Temperature outer layer (K)

!HGEN1=5000  !Heat generation
!HGEN2=5000
!HGEN3=5000
!HGEN4=5000
!HGEN5=5000
!HGEN6=5000
!HGEN7=5000
!HGEN8=5000
!HGEN9=5000

*ELSE
!******READ INPUT DATA FROM FILES**************
*DIM,out,ARRAY,1
*VREAD,out(1),Temp_MatL,TXT
(F13.2)
Tempout=out(1)

*DIM,condu,ARRAY,1
*VREAD,condu(1),KXX_MatL,TXT
(F13.2)
KXXa=condu(1)
*DIM,RHOa,ARRAY,1
*VREAD,RHOa(1),RHO_MatL,TXT (F13.0)
DENSa=RHOa(1)

*DIM,HGEN1a,ARRAY,1
*VREAD,HGEN1a(1),HGEN1_MatL,TXT (F13.0)
HGEN1=HGEN1a(1)

*DIM,HGEN2a,ARRAY,1
*VREAD,HGEN2a(1),HGEN2_MatL,TXT (F13.0)
HGEN2=HGEN2a(1)

*DIM,HGEN3a,ARRAY,1
*VREAD,HGEN3a(1),HGEN3_MatL,TXT (F13.0)
HGEN3=HGEN3a(1)

*DIM,HGEN4a,ARRAY,1
*VREAD,HGEN4a(1),HGEN4_MatL,TXT (F13.0)
HGEN4=HGEN4a(1)

*DIM,HGEN5a,ARRAY,1
*VREAD,HGEN5a(1),HGEN5_MatL,TXT (F13.0)
HGEN5=HGEN5a(1)

*DIM,HGEN6a,ARRAY,1
*VREAD,HGEN6a(1),HGEN6_MatL,TXT (F13.0)
HGEN6=HGEN6a(1)

*DIM,HGEN7a,ARRAY,1
*VREAD,HGEN7a(1),HGEN7_MatL,TXT (F13.0)
HGEN7=HGEN7a(1)

*DIM,HGEN8a,ARRAY,1
*VREAD,HGEN8a(1),HGEN8_MatL,TXT (F13.0)
HGEN8=HGEN8a(1)

*DIM,HGEN9a,ARRAY,1
*VREAD,HGEN9a(1),HGEN9_MatL,TXT (F13.0)
HGEN9=HGEN9a(1)

*ENDIF

ET,1,SOLID87
MPTEMP,,,,,,
MPDATA,KXX,1,,KXXa
MPDATA,DENS,1,,DENSa
!MPDATA,QRATE,1,,5
MPDATA,KXX,2,,KXXa
MPDATA,DENS,2,,DENSa
!MPDATA,QRATE,2,,50
MPDATA,KXX,3,,KXXa
MPDATA,DENS,3,,DENSa
!MPDATA,QRATE,3,,500
MPDATA,KXX,4,,KXXa
MPDATA,DENS,4,,DENSa
!MPDATA,QRATE,4,,5000
MPDATA,KXX,5,,KXXa
MPDATA,DENS,5,,DENSa
!MPDATA,QRATE,5,,50000
MPDATA,KXX,6,,KXXa
MPDATA,DENS,6,,DENSa
!MPDATA,QRATE,6,,5
MPDATA,KXX,7,,KXXa
MPDATA,DENS,7,,DENSa
!MPDATA,QRATE,7,,50
MPDATA,KXX,8,,KXXa
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!MPDATA,QRATE,8,,500
MPDATA,KXX,9,,KXXa
MPDATA,DENS,9,,DENSa
!MPDATA,QRATE,9,,50000
SPH4, ,4,4,2
SPH4, ,4,2,4,4
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SPH4, ,<CR>
SPH4, ,4,8,5
SPH4, ,5,6
SPH4, ,6,7
SPH4, ,7,8
SPH4, ,8,9
/CPLANE,1
/ANG,1,30,XS,1
/REP,FAST
/TYP,1,5
VSEL, ,1
VATT, 1, 1, 0
VSEL, 2
VATT, 2, 1, 0
VSEL, 3
VATT, 3, 1, 0
VSEL, 4
VATT, 4, 1, 0
VSEL, , , 5
VATT, 5, 1, 0
VSEL, , , 6
VATT, 6, 1, 0
VSEL, , , 7
VATT, 7, 1, 0
VSEL, , , 8
VATT, 8, 1, 0
VSEL, , , 9
VATT, 9, 1, 0

!*

!*
MSHKEY,0
MSHAPE,1,3d
SMRTSIZE,8
VSEL, , , ALL
!*
VMESH,ALL

!*
DA,33,TEMP,Tempout
DA,34,TEMP,Tempout
BFV,1,HGEN,HGEN1
BFV,2,HGEN,HGEN2
BFV,3,HGEN,HGEN3
BFV,4,HGEN,HGEN4
BFV,5,HGEN,HGEN5
BFV,6,HGEN,HGEN6
BFV,7,HGEN,HGEN7
BFV,8,HGEN,HGEN8
BFV,9,HGEN,HGEN9
NUMMRG,ALL, , , , LOW
NUMCMP,NODE

FINISH
/SOL
/STATUS,SOLU
SOLVE
FINISH
/POST1
!*
/EFACET,1
PLNSOL, TEMP,, 0

*get,NNODES,node,,num,max
!NNODES=5
*DIM,TT,ARRAY,(NNODES),1
*DO,I,1,(NNODES),1
*GET,TEMP%I%,NODE,%I%,TEMP
TT(I,1)=TEMP%I%
*ENDDO

/*INPUT,ansuitmp
 *
*CREATE,ansuitmp
*CFOPEN,'TEMPERATURA','TXT',''
*VWRITE,TT(1,1), , , , , , , , , (F22.15)
*CFCLOSE
*END

/RGB,INDEX,100,100,100, 0
/RGB,INDEX, 80, 80, 80,13
/RGB,INDEX, 60, 60, 60,14
/RGB,INDEX, 0, 0, 0,15
/REPLOT
ANNEX III: MATLAB INTERFACE

% INPUT DATA
KXX=35.30 % Conductivity (W/mK)
density=11.34; % Density (kg/m3)
ZZZ=082 % Atomic number of the element
sourceint=1.97e19 %source intensity (sourceparticle/s)
Temp=278.15 %Temperature outer layer in Kelvin

% *****WRITE INPUT DATA TO FILES************
fileid=fopen('29.txt','r');
if fileid == -1
    fprintf('Error')
else
    i=1;
    while ~feof(fileid)
        newline=fgetl(fileid)
        document(i).line=newline
        i=i+1;
    end
result=fclose(fileid);
if result~=0
    fprintf('Error')
end

fileid = fopen('33.txt','wt');
header='MESSAGE: DATAPATH C:\MCNP\MCNP_DATA\';
fprintf(fileid,'%s
',header)
fprintf(fileid,'%s
',name);
fprintf(fileid,'%3.0f
',source);
for i=1:9
    newData = [i+1 1]; %cell number and material card
    newData2 = [i-(i+1)]; %geometry
    fprintf(fileid,'%1.0f %1.0f %3.2f %1.0f %1.0f
', newData, density,newData2);
end
for i=13:55
    fprintf(fileid,'%s
',document(i).line)
end
fprintf(fileid,'%s','fm4 ')
fprintf(fileid,'%s\n',sourceint);
factor=1.6E-13*sourceint*density; %MeV/g*source particle -> W/cm^3
fprintf(fileid,'%s\n',fm6')
material='M1'
fprintf(fileid,'%s\n',material);
material='M1'

% *****RUN MCNP ************
comando1=['cd C:\Users\Laura\Desktop\Exercises MCNP'];
dos(command1);
s1='C:\MCNP\MCNP_CODE\bin\mcnp6.exe ';
input='i=33.txt ';
s2='n=run33_'
comando2=[s1 input s2];
dos(comando2);

% ******RUN ANSYS **********

% % CHECK IF RUN BATCH IS SET TO 1 IN FILE BEAM.INP
% %****************************************************************************

% INPUT DATA FOR ANSYS
fileid=fopen('run33_o','r');
if fileid == -1
    fprintf('Error')
else
    i=1;
    while ~feof(fileid)
        newline=fgetl(fileid)
        document2(i).line=newline
        i=i+1;
    end
end
result=fclose(fileid);
if result~=0
    fprintf('Error')
end

for i=1:28
    line2=document2(4283);
    cell2=str2num(line2.line(1:28))*1000000; %convert to number and W/m^3
    line3=document2(4286);
    cell3=str2num(line3.line(1:28))*1000000;
    line4=document2(4289);
    cell4=str2num(line4.line(1:28))*1000000;
    line5=document2(4292);
    cell5=str2num(line5.line(1:28))*1000000;
    line6=document2(4295);
    cell6=str2num(line6.line(1:28))*1000000;
    line7=document2(4298);
    cell7=str2num(line7.line(1:28))*1000000;
    line8=document2(4301);
    cell8=str2num(line8.line(1:28))*1000000;
    line9=document2(4304);
    cell9=str2num(line9.line(1:28))*1000000;
    line10=document2(4307);
    cell10=str2num(line10.line(1:28))*1000000;
end

% ******WRITE INPUT DATA TO FILES***********
rho=density*1000;
fid = fopen('KXX_MatL.txt','w');
fprintf(fid,'%13.2f\n',KXX);
close(fid);
 fid = fopen('RHO_MatL.txt','w');
fprintf(fid,'%13.0f\n',rho);
close(fid);
 fid = fopen('HGEN1_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell2);
close(fid);
 fid = fopen('HGEN2_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell3);
close(fid);
fclose(fid);
fid = fopen('HGEN3_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell4);
fclose(fid);
fid = fopen('HGEN4_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell5);
fclose(fid);
fid = fopen('HGEN5_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell6);
fclose(fid);
fid = fopen('HGEN6_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell7);
fclose(fid);
fid = fopen('HGEN7_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell8);
fclose(fid);
fid = fopen('HGEN8_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell9);
fclose(fid);
fid = fopen('HGEN9_MatL.txt','w');
fprintf(fid,'%13.0f\n',cell10);
fclose(fid);
fid = fopen('Temp_MatL.txt','w');
fprintf(fid,'%13.2f\n',Temp);
fclose(fid);

% *****RUN ANSYS IN BATCH MODE*************
entrada='shieldingsphere.inp';
s1="C:\Program files\ANSYS Inc\v171\ansys\bin\winx64\ansys171.exe" -b -i ";
s2=' -o out.out';
comando=[s1 entrada s2];
dos(comando);

% *****RESULTS*****
fid = fopen('Temperatura.txt','r');
D = textscan(fid, '%f%f%f%f%f', 'HeaderLines',1, 'CollectOutput',1);
FileMax = max(D{:}(:));
fclose(fid);
fid = fopen('Maxtemp.txt','w');
fprintf(fid,'%13.0f\n',FileMax);
fclose(fid);