Final degree work
Degree in industrial technologies engineering

Study of the tritium production in a 1-D blanket model with Monte Carlo methods

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Abstract

In this work a method to collapse a 3D geometry into a mono dimensional model of a fusion reactor blanket is developed and tested. Using this model, neutron and photon fluxes and its energy deposition will be obtained with a Monte Carlo code. This results will allow to calculate the TBR and the thermal power of the blanket and will be able to be integrated in the AINA code.
Acknowledgements

Thanks to the Consejo de Seguridad Nuclear of Spain which gave financial assistance.

Thanks to the FEEL staff specially Alexia Sergeant which always was up to help with questions and Marco Fabbri which codes were very useful to understand the software and the blanket model.

Thanks to the professor Javier Dies who introduced me in this work and special thanks to the professor Alfredo de Blas who invested an enormous quantity of hours and effort to teach me the MCNP code, preparing tutorials, models and explanations, helping with the code errors and taking care that I correctly learned and understood the fundamental physics related to this work.
Index

Abstract ii
Acknowledgements iii
Index iv
List of Figures vii
List of Tables ix
Symbols xi

1 Objectives and project’s scope 1
  1.1 Motivation ................................................................. 1
  1.2 Scope of the project ................................................... 1
  1.3 Objectives ............................................................... 2

2 Introduction 3
  2.1 Nuclear Fusion Fundamentals ........................................... 3
  2.2 The Blanket ........................................................... 3
  2.3 The WCSB blanket ..................................................... 4
  2.4 MCNP code introduction .............................................. 4

3 WCSB blanket modelization 7
  3.1 The WCSB blanket model .............................................. 7
  3.2 The layers ............................................................ 7
    3.2.1 The steel components ............................................ 7
    3.2.2 The coolant .................................................... 8
    3.2.3 The breeder ................................................... 9
    3.2.4 First wall .................................................... 9
  3.3 Position of the layers ............................................... 9
  3.4 MCNP modelization .................................................. 11
    3.4.1 Surface card .................................................. 11
    3.4.2 Material card ................................................ 12
    3.4.3 Cell card .................................................... 13
    3.4.4 Mode card ................................................... 14
    3.4.5 Source card ................................................ 14
    3.4.6 Tally card ................................................... 15
Index

3.4.7 Number of simulations ........................................ 16

4 Results ......................................................... 17
  4.1 Presentation and units ........................................ 17
  4.1.1 Y-axis units ................................................ 17
  4.1.2 X-axis units ................................................ 18
  4.2 Small section simulations .................................... 18
  4.2.1 No boundary conditions ................................... 18
  4.2.2 Specular and white boundary conditions ............... 21
  4.3 Big section simulations ...................................... 23
  4.3.1 No boundary conditions ................................... 24
  4.3.2 Specular and white boundary conditions ............... 25
  4.4 Section comparison with boundary conditions ............ 26
  4.5 Chosen model ................................................. 28
  4.6 TBR .......................................................... 29
  4.7 Material libraries ............................................ 30

5 Budget ......................................................... 33

6 Conclusions and future work .................................... 35
  6.1 Conclusions .................................................. 35
  6.2 Future work .................................................. 35

A MCNP chosen model code ....................................... 37

Bibliography ....................................................... 43
List of Figures

3.1 Small section blanket view .............................................. 11
4.1 Neutron tracks on a small section blanket ............................ 19
4.2 Neutron flux, small section, no boundary conditions ............... 19
4.3 Neutron flux by energy ranks, small section, no boundary conditions .... 20
4.4 Neutron energy deposition, small section, no boundary conditions .......... 20
4.5 Photon flux and energy deposition, small section, no boundary conditions .... 21
4.6 Neutron flux depending on boundary conditions, small section .......... 22
4.7 Comparison between specular and white boundary condition with no boundary conditions, small section ..................................... 22
4.8 Photon flux, small section, all boundary conditions ................ 23
4.9 Photon energy deposition, small section, all boundary conditions ....... 23
4.10 Neutron flux section comparison, no boundary conditions ............... 24
4.11 Neutron energy deposition section comparison, no boundary conditions .... 24
4.12 Photon flux and energy deposition section comparison, no boundary conditions .... 25
4.13 Neutron flux depending on boundary conditions, big section ............. 25
4.14 Neutron energy deposition depending on boundary conditions, big section .... 26
4.15 Photon flux and energy deposition, big section, all boundary conditions .......... 26
4.16 Neutron flux, section comparison, white boundary condition ........... 27
4.17 Neutron flux, section comparison, specular boundary condition .......... 27
4.18 Neutron energy deposition and photon flux and energy deposition, section comparison (specular) .......................................................... 28
4.19 Neutron tracks on a big section blanket ................................ 29
4.20 Neutron flux by energy ranks, small section, no boundary conditions .... 29
4.21 MCNP default library and JEFF library comparison .................. 30
List of Tables

3.1 Steel layer mass composition ............................................. 8
3.2 Coolant layer atomic composition ....................................... 8
3.3 Breeder layer mass composition ......................................... 9
3.4 Li$_2$TiO$_3$ and Be$_{12}Ti$ mass composition ............................ 9
3.5 Natural abundance of tungsten ............................................ 9
3.6 Order and width of the layers ............................................ 10
4.1 TBR by layer ..................................................................... 30
### Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TBR</td>
<td>Tritium Breeding Rate</td>
</tr>
<tr>
<td>ITER</td>
<td>Nuclear fusion reactor of first generation being building nowadays</td>
</tr>
<tr>
<td>WCSB</td>
<td>Water Coolant Solid Breeder</td>
</tr>
<tr>
<td>MCNP</td>
<td>Monte Carlo N-Particles code</td>
</tr>
<tr>
<td>FEEL</td>
<td>Fusion Energy Engineering Laboratory, ETSEIB, UPC</td>
</tr>
<tr>
<td>AINA</td>
<td>Fusion reactor safety code developed at the FEEL</td>
</tr>
<tr>
<td>DEMO</td>
<td>Nuclear fusion reactor of second generation being planned nowadays</td>
</tr>
<tr>
<td>IFERC</td>
<td>International Fusion Energy Research Center</td>
</tr>
<tr>
<td>Tally</td>
<td>Data results specification of the MCNP</td>
</tr>
</tbody>
</table>
Chapter 1

Objectives and project’s scope

1.1 Motivation

In the framework of the FEEL studies this work has an important safety branch. The main motivation of the project is to find a proper way to collapse the geometry of a blanket into a one dimension model in order to allow its results to be integrated into the AINA code for safety studies developed at the FEEL. This work pretends to obtain the neutron flux profile and calculate its energy deposition and the Tritium Breeding Rate of the blanket too. As the tritium is one of the few actually dangerous materials if not the most in a nuclear fusion plant, it is important to know how much of it is produced. Not only for the auto-maintenance combustible question but to have an estimation of how much of it could be introduced in the atmosphere in case of an accident.

The results can be useful for the final Master’s project “Development of model of tritium insccatarium for safety studies for AINA codes for DEMO and ITER reactors” of Alexia Sergeant, and for the PhD thesis of Marco Fabbri, both of them related to the FEEL.

1.2 Scope of the project

The main body of the work will consist on the blanket modelization and simulation using the MCNP5 code. The results offered by this program will be physically interpreted and ready to be verified with deterministic codes. Different material libraries will be tested in order to discover if this changes the results obtained.

The simulations will be focused in a specific type of blanket, the WCSB that is one of the blankets which are being considered for the japanese DEMO reactor.
1.3 Objectives

- Collapse the blanket model in one dimension.
- Obtain the neutronic fluxes through a blanket so they will be able to be integrated to the AINA code.
- Obtain the TBR of a blanket.
- Obtain other data as neutronic energy deposition, photon fluxes and its energy deposition.
- Test different material libraries.
- Provide a physical explanation and understanding of the results.
Chapter 2

Introduction

2.1 Nuclear Fusion Fundamentals

A nuclear fusion plant is a kind of nuclear plant that receive the energy coming from the loss of mass of nuclear fusion reactions. The most efficient reaction and the one that most of the fusion reactors try to achieve is the next:

\[ H_2^+ + H_3^+ \rightarrow He^{4}(3.5\text{MeV}) + n(14.1\text{MeV})[1] \] (2.1)

The combustibles of the reaction are two isotopes of hydrogen. Deuterium and tritium fuse generating an alpha particle \((He^{2+})\) and a high energy neutron. As the mass of the products of the reaction is lower than the combustible, the energy associated to this mass loss is invested as cinematic energy of the alpha particle and the neutron.

Of the 17.6 MeV produced in each reaction, 3.5 MeV are carried by the alpha that will interact with the plasma heating it which will help to maintain the fusion conditions. The other 14.1 MeV are carried by the neutron which will escape from the plasma and will deposit this energy on the blanket by slow down neutron interactions.

2.2 The Blanket

The blanket comprehends the walls and systems that face the plasma and its radiation. Despite being the first physical barrier facing the plasma it doesn’t contain it, the confinement of the plasma is made through strong electromagnetic fields. The blanket has other functions all of them of big importance for the safety and sustainability of the reactor:

- **Capture the energy and radiation of the plasma.** The blanket acts as a radiation shield avoiding that any ionizing radiation exits its walls and, by neutronic and other
interactions, transform the energy of neutrons and photons into heat. This heat has to be evacuated by a refrigeration system. This system could use this energy to produce steam and therefore electric energy through a turbine.

- **Produce tritium.** As one of the main combusters of the fusion reactions is tritium which is a very rare and very expensive to produce, it is very important to produce enough of it to maintain the reactions despite the losses it can be produced during the feedback cycle. This production is based on a neutronic reaction like:

\[ n(\text{slow}) + Li \rightarrow He^4 + H^3 + 4.8MeV[1] \]  

- **Avoid too high energies of the plasma.** The first wall facing the plasma is made of a material specifically chosen by its melting temperature and other characteristics that will make it lose some quantity of material that will mix in the plasma if some temperature is reached. The high atomic number of this material will increase the bremsstrahlung radiation very fast, turning off the fusion reactions before any system is damaged.

### 2.3 The WCSB blanket

With the ITER reactor under construction the investigation over materials and fusion technologies is centered on the development of the second generation fusion reactors, DEMO.

WCSB is one of the possible blanket models for the japanese version of DEMO that are being considered. This work is centered on this specific type of blanket which sets the materials of the walls, the type of refrigeration it uses and the way to produce tritium.

WCSB is an acronym for Water Coolant Solid Breeder. It has a width of 60 cm and consists basically on a first wall made of tungsten, different components made of steel, breeder sections where the tritium is produced and refrigeration pipes.[2]

The main characteristics of this blanket type are:

- The coolant used is high-pressure water.
- The tritium is produced with solid breeder materials as Li ceramics like \( Li_2TiO_3 \).
- The neutron multipiers are based on Be.

### 2.4 MCNP code introduction

At this work the MCNP5 code is used. This code has been developed at Los Alamos National Laboratory which started to work on it at the 1950’s. MCNP is an acronym for Monte Carlo N-Particles. It is an estocastic code very extended and used.
Unlike other codes that are based on deterministic methods and solve the simulations using directly the physical equations, MCNP simulate the life of a particle a big number of times (stories).[3]

When following the travel of a particle the code decide if it has an interaction or a reaction randomly based on its probability to happen. The resulting direction after an interaction is randomly selected too.

After simulating thousands stories we have a good approximation of the real behavior of the system. But as every amount of estocastic phenomenons, the results have an error due to the variance. The bigger the number of stories, the lower will be the variance, therefor the error.
Chapter 3

WCSB blanket modelization

3.1 The WCSB blanket model

The blanket is a complex structure which contains different materials and systems. It has steel components, breeders where the tritium is generated, tritium extraction systems, refrigerating systems...

As the model is mono-dimensional an homogenization must be done. All these systems and material mixes will be collapsed in layers so the blanket properties will only change in one direction. Each of these layers consist in a mix of materials that represents a component of the blanket.

The data of the specific materials and its quantity at every layer as well as its width is provided by the IFERC, responsible man: Youji Someya, from the Japan Atomic Energy Agency.

3.2 The layers

This model has four different types of layers depending on the mix of the materials, but the same type of layer can have different widths. These layers represent the first wall, steel components, the breeders and the water refrigeration system.

3.2.1 The steel components

This layer consists in an alloy of steel known as F82H. As the blanket contains different components made of steel (like the refrigeration pipes), the way to collapse them in the mono dimensional model is to add steel layers along the blanket. All the materials of the alloy are the natural isotope mix of each element with the exception of the manganese that is pure $^{55}Mn$ and the carbon which is all $^{12}C$. 
The composition of this alloy can be seen at the Table 3.1. The main elements of the layer are iron, tungsten and chromium. It has a density of 7780 $\text{kg m}^{-3}$.

### 3.2.2 The coolant

This layer represents the water used for the refrigeration. This water is under a pressure of 15.5 MPa and its average temperature is about 300$^\circ$C with a density of 742.8 $\text{kg m}^{-3}$.

This is the only layer that will entry its composition data to the program as an atomic composition instead of a mass composition.

<table>
<thead>
<tr>
<th>H$_2$O</th>
<th>Atomic composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>2</td>
</tr>
<tr>
<td>O</td>
<td>1</td>
</tr>
</tbody>
</table>

**Table 3.2: Coolant layer atomic composition**
3.2.3 The breeder

The breeder layer is a mix of $Be_{12}Ti$ (neutron multiplier), $Li_2TiO_3$ (tritium producer) and $He$, the total density of the mix is $1840 \frac{kg}{m^3}$. The proportion of each one in the layer is the next:

<table>
<thead>
<tr>
<th>Material</th>
<th>Composition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Li_2TiO_3$</td>
<td>16.0</td>
</tr>
<tr>
<td>$Be_{12}Ti$</td>
<td>64.0</td>
</tr>
<tr>
<td>$He$</td>
<td>20.0</td>
</tr>
</tbody>
</table>

Table 3.3: Breeder layer mass composition

The proportion of elements of the mixes is the next:

<table>
<thead>
<tr>
<th>$Li_2TiO_3$ Composition (%)</th>
<th>$Be_{12}Ti$ Composition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^7Li$</td>
<td>44.30</td>
</tr>
<tr>
<td>$^6Li$</td>
<td>1.30</td>
</tr>
<tr>
<td>$^8Li$</td>
<td>10.0</td>
</tr>
<tr>
<td>$O$</td>
<td>44.4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$Be_{12}Ti$ Composition (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Be$</td>
</tr>
<tr>
<td>$Ti$</td>
</tr>
</tbody>
</table>

Table 3.4: $Li_2TiO_3$ and $Be_{12}Ti$ mass composition

3.2.4 First wall

This is the only layer that appears only once in the model. Consists on a thin film of 0.02 cm entirely made of tungsten. It has a density of $19300 \frac{kg}{m^3}$.

For the simulation it has been considered the tungsten as a mix of its isotopes in the same proportion as it is found in nature:

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Natural abundance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{182}W$</td>
<td>26.5</td>
</tr>
<tr>
<td>$^{183}W$</td>
<td>14.3</td>
</tr>
<tr>
<td>$^{184}W$</td>
<td>30.6</td>
</tr>
<tr>
<td>$^{186}W$</td>
<td>28.4</td>
</tr>
</tbody>
</table>

Table 3.5: Natural abundance of tungsten

3.3 Position of the layers

The model consists on 40 layers of the different types shown before. After the first wall, the model follows the same pattern alternating between coolant and breeder always among steel layers. We can see this order and the width of each layer on the next table:
<table>
<thead>
<tr>
<th>Type of layer</th>
<th>Width (cm)</th>
<th>Total width (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Wall</td>
<td>2.00·10^{-2}</td>
<td>2.00·10^{-2}</td>
</tr>
<tr>
<td>Steel</td>
<td>4.09·10^{-1}</td>
<td>4.29·10^{-1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>5.82·10^{-1}</td>
<td>1.01</td>
</tr>
<tr>
<td>Steel</td>
<td>8.09·10^{-1}</td>
<td>1.82</td>
</tr>
<tr>
<td>Breeder</td>
<td>4.13</td>
<td>5.95</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>6.11</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>6.54</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>6.70</td>
</tr>
<tr>
<td>Breeder</td>
<td>5.40</td>
<td>1.21·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>1.23·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>1.27·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>1.29·10^{1}</td>
</tr>
<tr>
<td>Breeder</td>
<td>6.98</td>
<td>1.98·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>2.00·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>2.04·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>2.06·10^{1}</td>
</tr>
<tr>
<td>Breeder</td>
<td>9.76</td>
<td>3.04·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>3.05·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>3.09·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>3.11·10^{1}</td>
</tr>
<tr>
<td>Breeder</td>
<td>1.61·10^{1}</td>
<td>4.72·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>4.74·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>4.78·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>4.80·10^{1}</td>
</tr>
<tr>
<td>Breeder</td>
<td>4.28</td>
<td>5.22·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>5.24·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>5.28·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>5.30·10^{1}</td>
</tr>
<tr>
<td>Breeder</td>
<td>1.00</td>
<td>5.40·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>5.42·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>5.46·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>5.47·10^{1}</td>
</tr>
<tr>
<td>Breeder</td>
<td>1.00</td>
<td>5.57·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>5.59·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>4.24·10^{-1}</td>
<td>5.63·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.65·10^{-1}</td>
<td>5.65·10^{1}</td>
</tr>
<tr>
<td>Breeder</td>
<td>1.00</td>
<td>5.75·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>9.72·10^{-1}</td>
<td>5.85·10^{1}</td>
</tr>
<tr>
<td>Coolant</td>
<td>2.56·10^{-1}</td>
<td>5.87·10^{1}</td>
</tr>
<tr>
<td>Steel</td>
<td>1.27</td>
<td>6.00·10^{1}</td>
</tr>
</tbody>
</table>

Table 3.6: Order and width of the layers

A picture showing this layer organization have been obtained with the Visual Editor of the MCNP.
3.4 MCNP modelization

The data of the model is introduced in the MCNP through surfaces cards, material cards and cell cards. The simulation mode, the particle source and the results cards need to be set too.

The software works in a three dimensional space (XYZ). The direction of the particles will follow the longitudinal axis of the blanket which will be the Y axis.

The section of the blanket will be rectangular in order to make it stackable with other identical blankets so we study the fluxes in a blanket of infinite section.

3.4.1 Surface card

The surfaces of the model consists in series of Y-planes that represents the limits between the different layer types (surfaces from 1 to 40) and the X and Z planes that represent the limits of the chosen section (surfaces 41, 42, 43, 44 and 50).

The surface card of the model looks like this:

```
C
C Surfaces
1    PY    2.00E-02
2    PY    4.29E-01
3    PY    1.01E+00
4    PY    1.82E+00
5    PY    5.95E+00

...  
39   PY    5.87E+01
40   PY    6.00E+01
41   PZ    10
42   PZ    0
43   PX    0
44   PX    10
```
The first number indicates the surface number, later the direction of the normal vector to the plane is set and the normal distance of the plane to the origin is represented in centimeters as the last number.

### 3.4.2 Material card

At this card the different materials of the model are defined and classified through a number. The materials 1, 2, 3 and 4 represent the steel, the water used as coolant, the breeder and the tungsten used as first wall respectively.

The material card of this model looks like this:

```plaintext
C Materials
C
C Steel
C
m1 26054.31c -5.13E-2
  26056.31c -8.06E-1
  26057.31c -1.86E-2
  26058.31c -2.48E-3
  24050.31c -3.65E-3
  24052.31c -7.04E-2
  24053.31c -7.98E-3
...
C
m2 ...
...
```

For every $m_i$ material we have to introduce all the different elements it contains in this way $ZZZ$AAA.abX. $ZZZ$ is the atomic number of the element and AAA it is the atomic mass number. abX specifies the library where the program will obtain the data of that element or isotope. If we want to introduce the mix of isotopes of an element according to its natural abundance we can introduce the element just once setting AAA=000 if this natural abundance data is on the abX library. If not, we need to introduce all the isotopes of the element separately.

If the abX command is omitted, the program will use its default library. For this work the JEFF library (a library focused on nuclear fusion technology) is used for all the materials. As this library doesn’t have the natural abundance of most of the elements a big number of isotopes had to be manually introduced and its proportions manually calculated.
The number that follows the isotope and library entry is the proportion of that element. If it has a positive value the software interprets it as an atomic proportion. If the value is negative the proportion is massic.

In this model the mass proportion is used always except for the material 2 \((m_2, \text{water})\) which uses the atomic proportion.

### 3.4.3 Cell card

This card defines the cells that divide the model specifying the surfaces that are the frontiers of it. To run the code all the infinite three dimensional space has to be defined by the cells. No point of the model can have no cell associated to it and no point of the model can be in more than one cell.

A cell is defined by its surface frontiers, the material it contains, its density and the type of particles that will be simulated.

This model will consist on 41 cells. The first 40 cells represent the 40 different layers of the blanket and the cell 41 represents the outside of the blanket where the particles will be lost if exit to it.

The cell card of this model looks like this:

```plaintext
C
C Cells
1 4 -19.3 50 -1 -41 42 43 -44 imp:n=1 imp:p=1
2 1 -7.88 1 -2 -41 42 43 -44 imp:n=1 imp:p=1
3 2 -0.7428 2 -3 -41 42 43 -44 imp:n=1 imp:p=1
4 1 -7.88 3 -4 -41 42 43 -44 imp:n=1 imp:p=1
5 3 -1.84 4 -5 -41 42 43 -44 imp:n=1 imp:p=1
6 1 -7.88 5 -6 -41 42 43 -44 imp:n=1 imp:p=1
7 2 -0.7428 6 -7 -41 42 43 -44 imp:n=1 imp:p=1
... 40 1 -7.88 39 -40 -41 42 43 -44 imp:n=1 imp:p=1
41 0 (-50):(50 -43 -40):(50 44 -40):(50 41 43 -44 -40):&
(50 -42 43 -44 -40):(40) imp:n=0 imp:p=0
C
```

The first number of each line defines the name of the cell. The second one sets the material of the cell using the number given at each material at the material card. The third number represents the density, in this work will be always in negative which means the density is treated as mass density in units of \(g/cm^3\).
Then the frontiers of the cell are defined using the names given at the surface card, this numbers being positive or negative indicates the sense of the surface which defines the cell.

The last entry indicates the particles that are allowed at the cell, at all the blanket neutrons and photons will be simulated except at the outside cell which is void.

At the line 41 we can see how the outside cell is defined as the combination of six different fully defined spaces ("," indicates union) to avoid to include a region of space in more than one cell.

### 3.4.4 Mode card

The mode card list all particles that will be simulated. The main objective of this simulations is to obtain the neutronic fluxes but the photons will be simulated too because its fluxes and energy deposit can be interesting as well.

The mode card of this model looks like this:

```plaintext
C
mode n p
C
```

### 3.4.5 Source card

This card sets the particle source. The type of particles and its energy and where this source is located.

A source card for this model looks like this:

```plaintext
C
sdef vec=0 1 0 dir=1 x=d1 y=0 z=d2 erg=14.1 par=n sur=50
si1 0 10
sp1 0 1
si2 0 10
sp2 0 1
C
```

The first line of the card defines the source as the first surface of the blanket which is the surface 50 (Y=0). The source will emit only neutrons, all of them with the energy resulting of the deuterium and tritium fusion, 14.1 MeV.

The *vec* and *dir* options means that all the neutrons are coming from the source following the Y direction.

The x, y and z options set the distribution of the surface where the neutrons will be emitted. In this example all the neutrons appear from a square of 10x10 cm on the Y=0 plane.
3.4.6 Tally card

The tally card specifies the data results the simulation will provide and its format. For these simulations we want to know the neutron and photon fluxes and energy deposition. Discriminating by energy ranks will be interesting too.

A tally card for this model looks like this:

\begin{verbatim}
C Tally
C f14:n 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 &
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 &
38 39 40
C f16:n 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 &
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 &
38 39 40
C f24:p 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 &
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 &
38 39 40
C f26:p 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 &
21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 &
38 39 40
C
\end{verbatim}

The first command of the tally sets the type of tally and the particle of study. The tallies x4 provide particle fluxes and the tallies x6 provide energy deposition.

After the type of tally there have to be set all the cells where the tally will give the data by the name given by the cell card. In this study we want to know about all the 40 layers of the blanket.

A line can be added to every tally to discriminate between energy ranks. The energy is expressed in $MeV$, this line would be added specifying its tally by its number and would look like this:

\begin{verbatim}
e14 0.1 1 15
\end{verbatim}

This would give 4 different sets of data, from 0 to 0.1 $MeV$, from 0.1 to 1, from 1 to 15 and the sum of all the three.
3.4.7 Number of simulations

The number of simulations the MCNP will run must be set manually. For all the simulations the source will emit one million particles as it is specified here:

C
nps 1e6
C
Chapter 4

Results

As one of the main objectives of this work is to achieve a correct mono dimensional collapse of the blanket model, it is interesting to run simulations using different sections sizes of the blanket. If the results doesn’t change in the non longitudinal axis of the model it could mean that the model is mono dimensional.

The following simulations will provide the neutron and photon fluxes through the blanket and its energy depositions as well. After deciding which model is appropiate the TBR will be calculated and a comparision beetwen libraries will be presented.

4.1 Presentation and units

Along this chapter numerous graphics will be presented, it is important to understand how they have been produced and what they represent.

4.1.1 Y-axis units

The main variable here is the flux ($\phi$) as it is used to calculate other data such as the energy depositions and the TBR by multiplying by its cross sections.

The flux is the distance travelled by all the particles of a certain kind inside a volume during a second. Its units are: \( \frac{cm}{mg/cm^3/s} \). In our code we won’t discriminate the flux by any direction, even the particles that are going backwards will increase the flux value.

The MCNP works always in relative units (per particle source). It means it gives the result of what a single source particle causes. Per exemple, a neutron coming from the source reacts with Be and a new neutron is produced, this neutron goes backwards while having elastic collisions until it is captured. The resulting flux will be the sum of the distance travelled by the source neutron and the distance travelled by the new neutron produced at the Be reaction without
depending on its direction, all this happened because of one single neutron coming from the source.

So the units for flux of the code instead of \( \frac{cm}{cm^3 \times s} \) actually are \( \frac{cm}{cm^3 \times n_s} \) in the case of the neutron flux. To have the correct flux we need to multiply this flux by the intensity of particles of the source per second:

\[
[\phi] = \left[ \frac{cm}{cm^3 \times n_s} \right] \times \frac{n_s}{s} = \left[ \frac{cm}{cm^3 \times s} \right] \quad (4.1)
\]

However, for this work we are not going to use the typical units of flux. As our objective is to see if the section of the model changes the results we can’t have the volume of the cell at the denominator of the expression or an increase of volum will result in lower values of flux.

The results are going to be presented using a flux that will consist on the distance travelled in a unit of distance instead of a volume. To cancel the influence of the section the results are multiplied by the value of the section of the model. We will keep the results in relative units, by this way, the units of flux of this project will be the result of multiplying the flux in relative units of the MCNP by the section of the model:

\[
[\phi] = \left[ \frac{cm}{cm^3 \times n_s} \right] \times cm^2 = \left[ \frac{cm}{cm \times n_s} \right] \quad (4.2)
\]

### 4.1.2 X-axis units

A single value is given to every cell of the model which represents a layer. As the layers have arbitrary widths the results at the graphic are presented using a X-axis layer based. Every horizontal distance value represent a different layer.

It is better to present the graphics this way instead of setting the values of distance of the layers to the X-axis because, as the widths will be increasing and decreasing arbitraly, it would create a false effect of distance proportion for equal X-distances at the graphic.

### 4.2 Small section simulations

For the first set of simulations the section of the blanket is set to a square of 10x10 cm.

#### 4.2.1 No boundary conditions

In these simulations all the particles that travel to the outside of the blanket are lost, this means that the blanket model is finite, it is not being stacked. The tracks of 1000 neutrons have been plot to have a graphic idea of what happens with the flux:
Figure 4.1: Neutron tracks on a small section blanket

The green lines represent the neutron tracks, we can see how the flux is concentrated at the beginning of the blanket.

Here we can see the neutron flux profile through the layers of the blanket:

Figure 4.2: Neutron flux, small section, no boundary conditions

This graphic shows an increase of neutron flux at the first 4 layers.

It is known that the $Be_{12}Ti$ part of the breeder sections acts as a neutron multiplier but as it can be seen at the Table 3.6 the first breeder layer is the layer number 5.

An explanation for this flux increase at the 4 first layers (tungsten, steel and water) could rely on a geometric matter. At the layer 5 the neutrons react with the $Be$ of the breeder and produce more neutrons. The neutrons that are produced there have a random initial flight direction, the same can happen to the neutrons that have other interactions with the matter. Then some of this particles travels backwards and, as the neutronic flux is not influenced by the direction or origin of the neutrons the result could be the increase seen at the figure 4.2.

In order to verify this explanation the flux graphic is divided by energy ranks:
The neutrons are divided in slow neutrons (energy under 0.1 MeV, blue line), fast neutrons (energy over 1 MeV, red line), intermediate neutrons (between 0.1 and 1 MeV, green line) and the sum of all the other three (the same flux than Figure 4.2, black line).

We can see how the maximum point of intermediate neutron flux is at the layer 5 where the first breeder is and where new slow or intermediate neutrons are supposed to be produced, the slow neutrons peak is close too. This graphic shows that there is not a big increase of fast neutrons flux, the increase we saw at Figure 4.2 is due to lower energy neutrons produced at the breeders or coming from collisions that changed its direction and energy.

The next graphic shows the neutron energy deposition through the blanket:

This graphic is easy to be physically understood. It can be seen how the neutrons deposit its energy more effectively depending on the type of layer where they are traveling.
The three highest peaks are at the water layers where the neutrons have a high rate of elastic collisions with small nucleus which means an important energy deposition, the breeder layers have maximum peaks too but not as high as the water and the steel layers have minimum peaks as it was expected as the elastic collisions at the alloy are with big nucleus and not too much energy is deposited by the neutrons.

The layer order of the table 3.6 is perfectly represented here as we see the pattern of low peaks (steel) between the high peaks of the water (neutron moderator) and the breeder layers.

The same tallies are obtained in these conditions for the photons:

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{photon_flux.png}
\includegraphics[width=0.5\textwidth]{photon_energy_deposition.png}
\caption{Phonon flux and energy deposition, small section, no boundary conditions}
\end{figure}

\subsection{Specular and white boundary conditions}

The MCNP5 offers two different kind of boundary conditions. Using it, the particles that arrive to the blanket walls are not lost but reflected to the inside of the blanket again. With this, the model approaches to an \emph{infinite blanket model}. It can be considered that the reflected particles are particles coming from a neighbour blanket, none of them is lost in the \emph{void}.

These conditions are set to the surfaces 41, 42, 43 and 44 of the surface card which represent the blanket walls.

- **Specular.** A particle track that hits a reflecting surface is reflected specularly. [3]

- **White.** A particle hitting a white boundary is reflected with a cosine distribution relative to the surface normal.[3] This means that the angles after the collision are not absolutely determined by the incident angle but they vary through an isotropic distribution.

This graphic shows the different neutron fluxes depending its boundary conditions:
The black line represents the same profile than Figure 4.2. As it was expected, the fluxes with boundary conditions are higher because no particles are lost to the void.

Expecting a behaviour similar to the last graphic the neutron energy deposition is represented depending on the type of boundary condition:

These graphics are coherent with the Figure 4.6. Obviously, the energy deposition without boundary conditions is lower.

With the white condition the neutron flux is higher than with the specular condition at the first layers, this represents a bigger energy deposition at the first layers with the white conditions.
At the last layers is the specular condition which has more neutron flux, we can see how only with the specular layer there is a significant energy deposition at these layers.

The photon flux and energy deposition has been calculated too:

![Graph showing photon flux and energy deposition](image)

**Figure 4.8:** Photon flux, small section, all boundary conditions

**Figure 4.9:** Photon energy deposition, small section, all boundary conditions

These graphics are coherent with the other figures of the section.

### 4.3 Big section simulations

A second set of simulations has been run with a section of 60x200 cm. This section is significantly bigger than the first one, from its comparison the final mono dimensional model will be chosen.
4.3.1 No boundary conditions

The new neutron flux profile can be compared with the profile obtained with the small section:

![Neutron flux section comparison, no boundary conditions](image1)

**Figure 4.10:** Neutron flux section comparison, no boundary conditions

It is clear that the no boundary conditions model is not mono dimensional.

The graphic shows a big difference between the two section models. The flux increase is higher and has its maximum at the layer 7 instead of the 5. The average flux is bigger too, this is surely due to a smaller number of particles lost as they have a bigger distance from the center of the blanket to its walls.

The energy deposition of the neutrons can be seen at the next graphic:

![Neutron energy deposition section comparison, no boundary conditions](image2)

**Figure 4.11:** Neutron energy deposition section comparison, no boundary conditions

The difference between the big section and the small is not as big for the neutron energy deposition as it is for the flux but it is still higher with the new section.
The comparison with the photons has been obtained too:

![Photon flux](image1)
![Photon energy deposition](image2)

**Figure 4.12:** Photon flux and energy deposition section comparison, no boundary conditions

As it was expected the values are higher with the bigger section.

### 4.3.2 Specular and white boundary conditions

The difference between the different boundary conditions sets for this section model is shown here:

![Neutron flux](image3)

**Figure 4.13:** Neutron flux depending on boundary conditions, big section

The graphic had to be divided in two subplots because the flux with specular boundary conditions is practically equal to the flux with white conditions. This is a good situation because it can mean that when the section is big enough like now, the different boundary conditions have the same result. This can be a good indication that the model is mono dimensional.
Despite the similarities between specular and white, both of them show a bigger neutron flux than the model without boundary conditions as it was expected.

As it happened at the Figure 4.13 this graphic had to be divide in two subplots. The neutron energy deposition is practically the same for the specular and white boundary conditions. Both of them having greater values than the model without the boundary conditions.

The same comparisons have been made with the photons:

4.4 Section comparision with boundary conditions

The comparison of the section 4.2.1 showed big difference between the small and big sections models without boundary conditions. It is clear that our final model needs a boundary condition
that avoid variations in the non longitudinal axis of the blanket.

We can see how the results change if we apply the same white boundary condition to both sections:

**Figure 4.16:** Neutron flux, section comparison, white boundary condition

Using the white boundary conditions the neutron fluxes of the small and big section models are
very similar although not the same. However the graphic shows an improvement of the mono
dimensional model compared to the model without boundary conditions.

If the specular boundary condition is applied to both sections the next neutron flux is obtained:

**Figure 4.17:** Neutron flux, section comparison, specular boundary condition
The results are so similar that is difficult to differentiate between the two different lines at the graphic. This is a good indication that the model achieve a mono dimensional property using the specular condition.

From now on this work will continue only using the specular boundary condition as it has been proved that it has the best mono dimensional performance. Here we can see the comparison between sections of the rest of results using the specular condition:

All the results are so similar we barely appreciate any difference between sections.

4.5 Chosen model

The final model chosen for the calculation of the TBR is the blanket with the 60x200 cm section (big section) using the specular boundary condition due its good performance showed at the earlier graphics. 1000 neutron tracks heve been plot to have a graphic idea of the flux.
Study of the tritium production in a 1-D blanket model with Monte Carlo methods

Figure 4.19: Neutron tracks on a big section blanket

It is interensting know the neutron flux discriminating by energy ranks.

Figure 4.20: Neutron flux by energy ranks, small section, no boundary conditions

The results are the expected, we can proceed.

4.6 TBR

A multiplier is add to the tally which calculates the neutron flux for the final model. Now the tally is programmed to calculate only at the breeder layers (5, 9, 13, 17, 21, 25, 29, 33 and 37).

As the reaction rate is the product of the cross section of the reaction and the particles flux, the multiplier represents the cross section of the reaction where the Li and a neutron produce one tritium atom so the result is the TBR of every breeder layer.
This TBR is a result in relative units. It gives the number of tritium atoms that are produced for every neutron the source emits.

The results are:

<table>
<thead>
<tr>
<th>Layer number</th>
<th>TBR</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>(3.30 \times 10^{-1})</td>
</tr>
<tr>
<td>9</td>
<td>(3.18 \times 10^{-1})</td>
</tr>
<tr>
<td>13</td>
<td>(3.01 \times 10^{-1})</td>
</tr>
<tr>
<td>17</td>
<td>(2.57 \times 10^{-1})</td>
</tr>
<tr>
<td>21</td>
<td>(1.63 \times 10^{-1})</td>
</tr>
<tr>
<td>25</td>
<td>(1.96 \times 10^{-2})</td>
</tr>
<tr>
<td>29</td>
<td>(4.68 \times 10^{-3})</td>
</tr>
<tr>
<td>33</td>
<td>(3.94 \times 10^{-3})</td>
</tr>
<tr>
<td>37</td>
<td>(2.62 \times 10^{-3})</td>
</tr>
</tbody>
</table>

Table 4.1: TBR by layer

The total TBR of the model is the sum of the TBR of every breeder: \(\text{TBR} = 1.4\). The usual values for the TBR that are wanted and obtained are between 1.05 and 1.2. The TBR obtained here is significantly higher although not an irrational value.

### 4.7 Material libraries

All this work have run with the JEFF library of materials, specifically the version JEFF 311. This library is very common at the nuclear fission and fusion studies. However it can be interesting test other libraries to see if it changes the results.

Here we can see a comparison of the neutron flux of the chosen model between the JEFF library and the MCNP5 default library:

![Figure 4.21: MCNP default library and JEFF library comparison](chart.png)
Other libraries were attempted to be tested but unfortunately there were some unidentified problems with its compilation.

Using the MCNP5 default library the flux is significantly bigger. A deeper study of the libraries could be interesting in the future.
Chapter 5

Budget

The salary of the student at practices recommended by the UPC is 8€/hour. The cost of the student have been calculated using this salary during the hours equivalent to the 12 credits of the final degree work.

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Price (€/u)</th>
<th>Quantity</th>
<th>Cost (€)</th>
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<td>1000,00</td>
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<td><strong>Total equipment cost</strong></td>
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<td><strong>1000,00 €</strong></td>
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</tbody>
</table>

<table>
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<th>Price (€/u)</th>
<th>Quantity</th>
<th>Cost (€)</th>
</tr>
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<tr>
<td>MatLab R2015a</td>
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<td><strong>Total licensing cost</strong></td>
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</table>

<table>
<thead>
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<th>Human resources</th>
<th>Cost (€/hora)</th>
<th>Hours</th>
<th>Cost (€)</th>
</tr>
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<td>360</td>
<td>2880</td>
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<tr>
<td><strong>Total H.H. R.R.</strong></td>
<td></td>
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<td><strong>2880 €</strong></td>
</tr>
</tbody>
</table>

**TOTAL** | 4129 €
Chapter 6

Conclusions and future work

6.1 Conclusions

The method to simulate a parallelepiped of rectangular section applying boundary conditions to its walls that act as this prism is stacked with other identical prisms has been tested and it seems to provide correct results for the specular boundary condition with the MCNP5 code. This method can be useful to collapse 3D geometries into monodimensional models.

The data of the mono dimensional collapse of the WCSB blanket from the IFERC have been used for the simulations and the neutron and photon flux profiles and energy deposition through the blanket have been obtained.

The TBR associated to this profile flux for this type of breeder have been calculated resulting in a generation of 1.4 tritium atoms for every neutron coming from the plasma. This value is reasonable but higher than the expected.

A comparison between the default library of the MCNP5 and the JEFF library have been made, it can be observed higher values of neutron flux using the default library.

This results are able to be integrated at the AINA code developed at the FEEL.

6.2 Future work

The results of this work should be verificated with other sources. A non estocastic but deterministic code like SCALE is a good candidate for this verification.

If it is possible, compare the results with other similar studies made by the investigators of the Japan Atomic Energy Agency.

A deeper study which explains the differences of the results between the different libraries could be interesting. Also prepare the libraries that didn’t work can be useful for future projects.
Appendix A

MCNP chosen model code

WCSB Big section, Specular boundary conditions

<table>
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6 | PY | 6.11E+00 |
7 | PY | 6.54E+00 |
8 | PY | 6.70E+00 |
9 | PY | 1.21E+01 |
10| PY | 1.23E+01 |
11| PY | 1.27E+01 |
12| PY | 1.29E+01 |
13| PY | 1.98E+01 |
14| PY | 2.00E+01 |
15| PY | 2.04E+01 |
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sp1 0 1
si2 0 200
sp2 0 1
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C Tallies
C
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    38 39 40
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