Tritium breeding simulation with Geant4

Alessandro Mancini

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Abstract

The purpose of this project is to simulate, with the Geant4 software, the production of neutrons generated by nuclear fusion inside a simplified tokamak inspired by ITER, to study the tritium breeding phenomenon and to obtain an estimate of the Tritium Breeding Ratio (TBR) for a simplified breeding blanket. The project is host in the following github repository: `https://github.com/jonni2/Geant4-Tokamak`

Tritium breeding is currently the best candidate process to produce tritium: one of the two fuels (together with deuterium) for future nuclear fusion reactors. The problem with tritium is that, unlike deuterium, is incredibly rare on Earth and has to be produced in some ways. The idea of tritium breeding is to use the neutrons generated by nuclear fusion itself to produce some tritium inside the fusion reactor, during its operation.

Because of this reason future fusion reactors will foresee the presence of a breeding blanket: a layer made of particular isotopes (most likely lithium) that, reacting with the neutrons, will produce the desired tritium. The Tritium Breeding Ratio (TBR) parameter is defined as the ratio between the number of tritium nuclei produced over the number of reagent neutrons and indicates how efficient the breeding reaction is. An ideal reactor requires TBR > 1 in order to have sufficient tritium to continue the operation.

In this project Geant4 has been used to design a simplified tokamak and its breeding blanket and to implement the physics of tritium breeding. Some simulations have been executed and the TBR has been evaluated for different ^{6}Li enrichments and breeding blanket designs: WCLL (Water Cooled Lithium Lead), HCPB (Helium Cooled Pebble Bed). The TBR showed to increase as the ^{6}Li enrichments increases; the beryllium layers in the HCPB design showed to increase the TBR; finally the WCLL design (implemented as pure PbLi) showed the highest TBR.

Contents

1 Introduction to nuclear fusion and tritium breeding

Nuclear fusion is a promising candidate energy source for future sustainable cities. As opposed to nuclear fission, fusion is a class of nuclear reactions in which light nuclei, brought to very high temperatures, can be fused together to form heavier nuclei and release thermal energy according to Einstein's equation $E = \Delta M c^2$; ΔM being the mass difference between reagents and products. Today the most promising and investigated fusion reaction is the one between the two isotopes of hydrogen **deuterium and tritium** (DT):

$$ {}^2_1\mathrm{D} + {}^3_1\mathrm{T} \rightarrow {}^4_2\mathrm{He}\ (3.5\mathrm{MeV}) + \mathrm{n}\ (14.1\mathrm{MeV}) $$

This reaction releases an energy of 17.6 MeV in the products: a neutron and an alpha particle. This energy translates to 337 TJ per kg of DT [7], to compare to $\sim$ 80 TJ/kg for conventional uranium fission and $\sim$ 50 MJ/kg for hydrocarbon combustion.
However this reaction has a **threshold**: the reagent DT mixture needs to be heated to a high temperature in order for the nuclei to overcome the Coulomb barrier and achieve a significative fusion rate. The reaction's cross section peaks around 70 keV, but because of quantum tunnelling effects it is not necessary to bring the DT reagents to such high temperatures; currently the aim is around 10-15 keV.
At such high temperatures the DT mixture becomes a plasma: an ionized gas where electrons are stripped from the nuclei. These hot thermonuclear plasmas have to be confined, increasing particle density n, in order to achieve a good fusion rate according to the equation:

$$ R_f \left[\frac{\#}{cm^3 \cdot s} \right] = \frac{n_D \cdot n_T}{4} < \sigma v > \quad (1) $$

where $n_{D/T}$ $[\#/cm^3]$ are the densities of deuterium and tritium nuclei and $< \sigma v >$ is the product of fusion cross section and reagents' velocities averaged with the velocity distribution function of the reagents (usually assumed as a maxwellian distribution) [4].
The confinement of the plasma can happen through different techniques: mainly *inertial confinement* and *magnetic confinement*. The former foresees the use of high power lasers on small solid DT targets, as done by the National Ignition Facility (NIF). The latter makes use of reactors with powerful magnetic fields to confine the gaseous DT mixture which has to be heated to keV temperatures.
This report focuses on **magnetic confinement fusion**.

The possibility to achieve commercial nuclear fusion as an energy source depends on some critical problems which are currently important research topics addressed by the numerous research centers all around the World:

- **plasma stability**: in magnetic confinement reactors the plasma manifests a great number of instabilities that degrade the fusion performance;
- **power exhaust**: fusion plasmas release high heat loads on the reactor's components, which require specific heat-resistant materials;
- **neutron tolerant materials**: in future reactors the high neutron flux will also require specific materials;

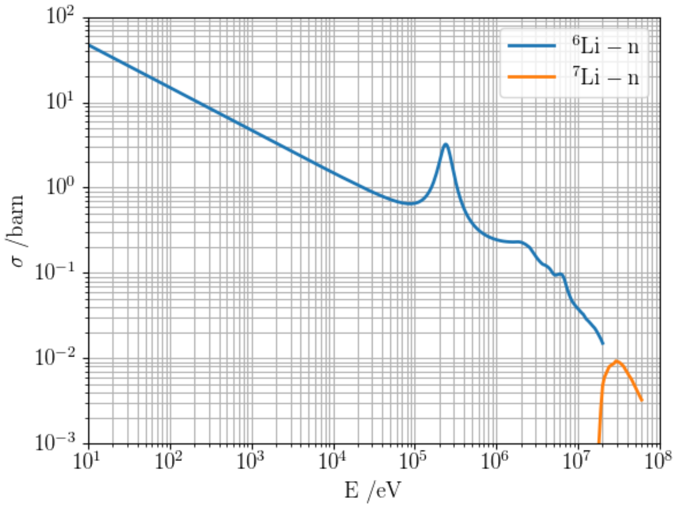

Figure 1: Energy dependent cross sections for the two tritium breeding reactions. The one with $^6_3$Li is far higher.

- **tritium self sufficiency**: tritium is an incredibly rare isotope on Earth, therefore a way to produce it has to be found.

This project in particular deals with this last problem: the tritium self sufficiency which is now, according to many, the biggest challenge for commercial nuclear fusion.
Tritium is in fact a very rare isotope on Earth, which is produced mainly by the interaction between cosmic rays and the atmosphere and by nuclear fission reactors. However the quantity of tritium produced, both naturally and artificially, will unlikely be sufficient for a future nuclear fusion power plant [3]. For this problem there are mainly two solutions:

- study some other fusion reactions which don't involve tritium;
- find a method to produce tritium.

Even if there are many research centers and private companies that are studying other fusion reactions the DT one is by now the best known and the one with the lowest threshold temperature, which makes it the *easiest* to use.
For this reason a way to produce tritium has to be developed. Currently the best proposal is to produce it inside the fusion reactor itself, by using particular nuclear reactions. The most promising is a reaction between the fusion-produced neutrons and lithium [8]:

$$\mathrm{n} + {}^6_3\mathrm{Li} \rightarrow {}^4_2\mathrm{He} + {}^3_1\mathrm{T} \ \ (+4.78\ \mathrm{MeV}) \tag{2}$$

$$\mathrm{n} + {}^7_3\mathrm{Li} \rightarrow {}^4_2\mathrm{He} + {}^3_1\mathrm{T} + \mathrm{n}' \ \ (-2.47\ \mathrm{MeV}) \tag{3}$$

This reaction would exploit the 14.1 MeV neutrons produced by fusion which, interacting with some materials containing lithium, would produce tritium. The reaction can happen both with the two natural isotopes of lithium; however $^7_3$Li is far more abundant than $^6_3$Li (92.4 % vs 7.6 %) and unfortunately the reaction cross section of $^7_3$Li is much lower than the one of $^6_3$Li, as shown in Fig. 1. For this reason and because the cross section with $^6_3$Li is higher at lower neutron energies lithium will probably require enrichment and neutrons will require moderation.

2 Breeding blanket

The aforementioned nuclear reaction between fusion neutrons and lithium is to be used in a so called **breeding blanket**: a specific layer in the fusion reactor which embeds some lithium alloys.
Up to now the best candidate fusion reactor is the **tokamak**: a doughnut-shaped machine with powerful magnetic coils to confine the plasma. There are several experimental tokamaks in the world but there has never been an extensive experimental program on tritium breeding. This will come with the ITER project (International Thermonuclear Experimental Reactor): a big tokamak now under construction in Cadarache, France.
ITER will have to prove, among the other goals, the **feasibility of tritium breeding** and breeding blankets. For this reason ITER will be equipped with some small modules, called **Tritium Breeding Modules** (TBM), which will simulate breeding blankets. This choice has been made in order to study different breeding technologies and understand which is the best. The ITER program foresees in fact the use of different breeding modules, the main ones being [1]:

- Helium Cooled Lithium Lead (HCLL): helium as coolant and liquid lithium-lead alloy (PbLi) as breeder;
- Helium Cooled Pebble Bed (HCPB): lithium ceramic pebbles (Li_4SiO_4) as breeder and helium as coolant;
- Water Cooled Lithium Lead (WCLL): liquid PbLi as breeder and water as coolant;
- Water Cooled Ceramic Breeder (WCCB): lithium ceramic with water as coolant;
- Dual Coolant Lithium Lead (DCLL): concept that uses both helium and water as coolants and PbLi as breeder;
- Helium Cooled Ceramic Breeder (HCCB): high pressure helium as coolant and lithium ceramic pebbles (like Li_4SiO_4) as tritium breeder, with beryllium pebbles as neutron multiplier.

After an extensive study with these TBMs future nuclear fusion reactors will embed an entire blanket made with some of these technologies. Fig. 2 shows the scheme of a potential tokamak fusion reactor with a breeding blanket and the tritium fuel cycle: tritium is supplied to the reactor and is extracted from the blanket after the tokamak's operation.

This project tried to implement and simulate, with the Geant4 software, a very simplified version of two of these technlogies: HCPB and WCLL. Different configurations and materials have been simulated and comparisons of the obtained TBR (Tritium Breeding Ratio) have been executed.

3 Geant4 program

Geant4 (`https://geant4.web.cern.ch/`) is a toolkit for the simulation of particles' interactions with matter, written in C++, object oriented and originally developed at CERN. It can be used for a great variety of applications: simulating radiation's interaction with matter, radioactive decays, particle accelerators, radioactive activation, gamma rays, radiobiology,

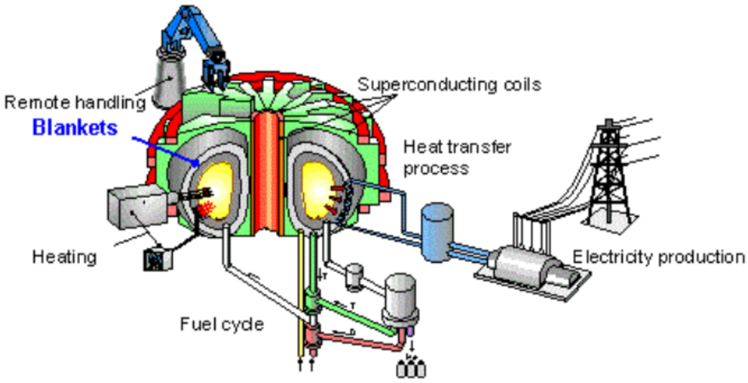

Figure 2: Scheme showing the breeding blanket and the tritium fuel cycle in a potential tokamak nuclear fusion reactor. Initial tritium is supplied to the reactor and new tritium is extracted from the breeding blanket. Ideally the tritium produced should be at least the same of the tritium supplied.

radiotherapy and hadron therapy and many more.
Geant4 is a Monte Carlo simulator: it tracks the history of every particle generated and it uses random numbers to evaluate the interactions between particles and matter. It can calculate several physical quantities of interest like the energy deposited by a charged particle, the number of photons and Cherenkov photons emitted and the radiation dose.
Geant4 offers the possibility to build custom geometries and materials to accurately simulate real objects; visualization of geometry and particles' trajectories is also possible with, among various possibilities, OpenGL.
In the following sections the main files in the project are discussed.

3.1 Geant4 program description

The project's source code can be found in the Github repository `https://github.com/jonni2/Geant4-Tokamak`, where also the compiling instructions with CMake can be found. The project requires Geant4 already installed or can be run with Docker from an image which already contains it.
The program takes in input the `run.mac` file which has to be written in the following way:

```
/run/beamOn N1
/run/beamOn N2
...
/run/beamOn Nn
```

where every line specifies the number of neutrons to generate during each simulation. The program runs n times and at the end of each simulation it writes on `outfile.txt` the Tritium Breeding Ratio (TBR) as the ratio of tritium atoms produced in the breeding blanket (see Sec. 3.4) over input neutrons:

$$TBR = \frac{\#T_{out}}{\#N_{in}} \tag{4}$$

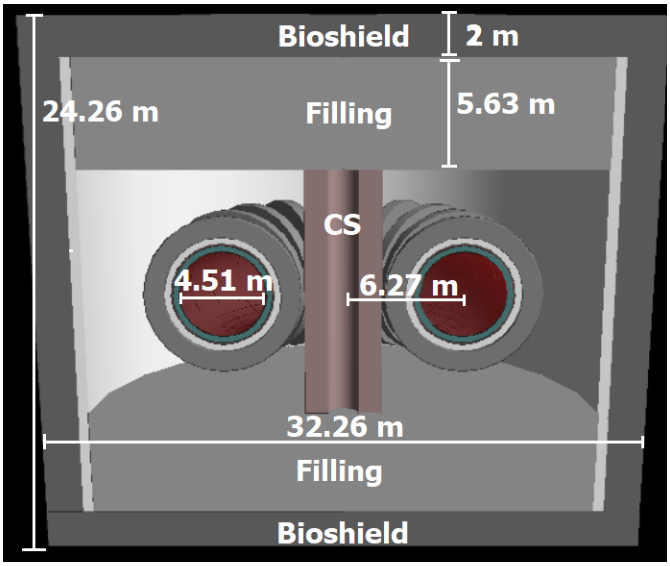

Figure 3: Geometrical model of the tokamak reactor implemented in the Geant4 simulation. The Central Solenoid (CS) and Bioshield are evidenced. *Filling* is a layer of mixed materials to simulate all the supports, instruments and cables that fill that area of the reactor. Some physical dimensions are evidenced.

3.2 Simulation geometry (files Construction.hh/cc)

In this project a model tokamak inspired by ITER has been implemented following the paper by Mohammad Mehdi Nasseri [6] which specifies the dimensions and materials of the model. The tokamak is simplified as a series of **cylindrical and toroidal layers** provided by the Geant4 classes `G4Tubs` and `G4Torus`. Every layer represents some component of the tokamak and is given a specific material. Materials in Geant4 are represented by the class `G4Material` and have a density (g/cm^3) and an isotopic composition. Fig. 3 shows an inside view of the reactor's geometry implemented with Geant4. Fig. 4 is a zoom of the torus' layers. All the layers and materials used are summarized in Tab. 1, where also the thickness of each layer is reported. All the materials have been taken and simplified from [6]. Two Geant4-defined materials have been used: `G4_Galactic` and `G4_Concrete`. The first is a material which is used to represent the vacuum space and it well fits to the tokamak's plasma, which has

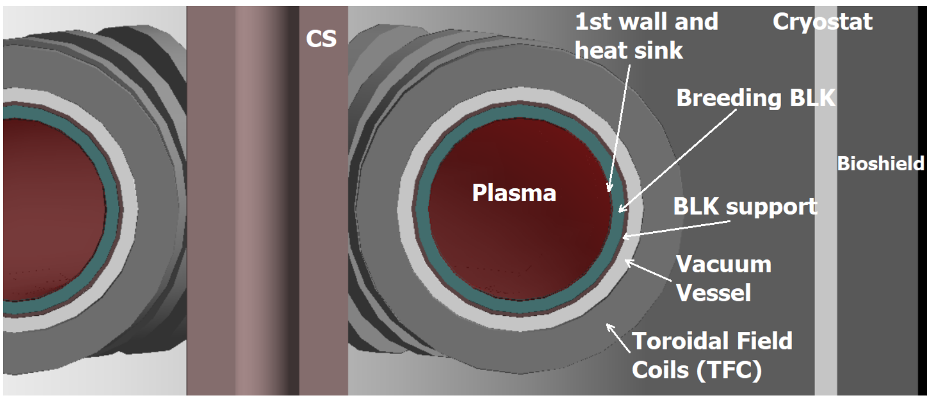

Figure 4: Zoom of the layers of the tokamak. CS is the Central Solenoid, BLK is the tritium breeding blanket.

Layer	**Shape**	**Material**	**Thickness**
Central Solenoid (CS)	Cylinder	Nb_3Sn: 45% Incoloy908: 50% Al_2O_3: 5%	120 cm
Plasma	Torus	G4_Galactic (vacuum)	Diam = 451 cm
1st wall	Torus	Tungsten	1 cm
1st wall heat sink	Torus	Copper: 98.8% Chrome: 1% Zirconium: 0.2%	2 cm
Breeding Blanket	Torus	Variable (HCPB, WCLL)	31 cm
Blanket support	Torus	SS316	10 cm
Vacuum Vessel	Torus	SS316	35.7 cm
Toroidal Field Coils (TFC)	Torus	Same as CS	100 cm
Cryostat	Cylinder	SS316	55 cm
Filling (x2)	Cylinder	SS316: 75% Copper: 15% G4_Concrete: 10%	Height = 563 cm
Lateral Bioshield	Cylinder	G4_Concrete	Height = 2426 cm
Top, bottom Bioshield	Cylinder	G4_Concrete	200 cm

Table 1: Material composition of the reactor's layers. SS316 is a type of Stainless Steel composed of 70% Fe, 17% Cr, 11% Ni and 2% Mo. Incoloy908 is a type of superalloy composed of 50% Ni, 40% Fe, 5% Cr, 5% Nb. G4_Galactic and G4_Concrete are two Geant4-defined materials to respectively simulate vacuum and concrete.

incredibly low density. The second represents concrete used in the radiation shield of the reactor.
For the Breeding Blanket more materials have been tried, as discussed in the next section.

3.3 Breeding blanket

As previously mentioned several blanket designs have been simulated in this project and some comparisons have been performed. One important parameter that has been included is the lithium enrichment fraction. Lithium is in fact the core element of every breeding blanket design: the breeding cross section is much higher for ^{6}Li than ^{7}Li (see Fig. 1) but the latter is way more abundant in nature than the former. Therefore lithium will be required to be enriched in ^{6}Li in a blanket's design.
In this Geant4 project the enrichment fraction can be passed as a double number at runtime when starting the program in the following way: `./Tokamak_Breeding run.mac 6Li%`
In the following section the results of several simulations are discussed: every blanket design has been simulated with 2 runs of 50000 neutrons each and with ^{6}Li enrichment of 0%, 7.5% (natural Li), 50% and 100%. All the results are reported in Tab. 2. All blankets have shown TBR = 0 with 0% ^{6}Li, therefore the results for this enrichment are not listed.

3.3.1 Pure PbLi blanket (WCLL)

The first design is inspired by a simplified Water Cooled Lithium Lead (WCLL) blanket. The 31 cm thick Breeding Blanket in Tab. 1 has been totally filled with PbLi (lithium lead): a liquid alloy made of lithium and lead. According to literature the density has been chosen as 9.8 g/cm^3 and the proportions are 20% Li and 80% Pb [5].

3.3.2 Pure Li_4SiO_4 blanket (HCPB)

The second simulated design is inspired by a simplified Helium Cooled Pebble Bed (HCPB) blanket. The 31 cm thick Breeding Blanket in Tab. 1 has been totally filled with lithium orthosilicate (Li_4SiO_4) whose density is 2.45 g/cm^3.

3.3.3 Li_4SiO_4 blanket with beryllium layers (HCPB)

Two variations of the previous design have been implemented: the first with one 5 cm thick beryllium layer in front of the breeding blanket; the second with two 5 cm thick beryllium layers and the Li_4SiO_4 breeding blanket sandwiched between them.
The 31 cm thick layer in Tab. 1 has therefore been divided into sublayers:

- design 1: 5 cm thick Be layer and 26 cm thick Li_4SiO_4 breeding blanket;
- design 2: 21 cm thick Li_4SiO_4 sandwiched between two 5 cm thick Be layer.

Beryllium is an important material in nuclear applications since it acts as neutron moderator and multiplier, therefore enhancing the TBR [2]. A very important difference in the TBR can be seen between the standard HCPB design and the ones with Be layers in Tab. 2.

BLK design	^{6}Li enrich (%)	Tritium Breeding Ratio (TBR)
WCLL (Pure PbLi)	7.5	1.301
	7.5	1.297
	50	1.411
	50	1.409
	100	1.410
	100	1.409
HCPB	7.5	0.840
	7.5	0.845
	50	1.012
	50	1.007
	100	1.055
	100	1.055
HCPB with front Be layer	7.5	0.964
	7.5	0.973
	50	1.135
	50	1.140
	100	1.187
	100	1.189
HCPB with two Be layers front/back	7.5	0.967
	7.5	0.974
	50	1.138
	50	1.143
	100	1.189
	100	1.186

Table 2: Main results of the simulations performed, each one with 50000 neutrons generated. It can be observed that the TBR increases cwhen the ^{6}Li enrichment increases, as expected. The Be layers proved to increase the TBR of the HCPB design (by $\sim$ 12-15%). The WCLL design showed the highest TBR.

3.3.4 Simulation results

The main results of the simulations are reported in Tab. 2. The first observation is that, in every blanket design, the TBR increases as the ^{6}Li enrichment increases, as expected. All the HCPB designs with natural lithium (7.5% ^{6}Li enrichment) have shown TBR $<$1, which must be avoided in order to guarantee a tritium self sufficiency for a reactor.
Furthermore the Be neutron multiplier layers have proven to be efficient in increasing the TBR (by $\sim$ 12-15%); however no particular difference has been observed between the HCPB with one Be layer and the HCPB with two Be layers.
The pure PbLi (simplified WCLL) design showed the highest TBR. However it must be mentioned that this design is incredibly simplified and not a good representative of a real WCLL blanket.

3.4 Sensitive Detector (files Detector.hh/cc)

Geant4 allows to define a volume in the simulation which acts as a Sensitive Detector. These kinds of volumes can be used to measure several quantities of interest during a particle interaction event with the volume itself.
In this project the Breeding Blanket itself has been chosen as the Sensitive Detector and its role is to detect tritium breeding reactions and count the number of tritium nuclei produced.
In order to do this the Geant4 class `G4VSensitiveDetector` and its method `ProcessHits()` have been used. Inside this method a counter `N_Tritium` increments every time a triton nucleus generated by a "neutronInelastic" process is detected.
At the end of the simulation the value of this counter is used in the `main()` function, together with the number of input neutrons (see Sec. 3.1), to calculate the Tritium Breeding Ratio.

3.5 Simulation physics (files PhysicsList.hh/cc)

These files are used to include the desired physics in the simulation. In particular the files `NeutronHPphysics.hh/cc` have been taken from the Geant4 example Hadr04. They are used to implement the physics of neutrons with energies up to 20 MeV.

3.6 Particle generator (PrimaryGeneratorAction.hh/cc, setup.mac)

The files `PrimaryGeneratorAction.hh/cc` are used to implement the kind of particles that are generated when the command `/run/beamOn` is called. In the case of this project neutrons are generated.
The kinetic characteristics and the angular distribution of the neutrons are set in the `setup.mac` file, with the `/gps/` commands ("General Particle Source"). In particular the neutrons are generated in all directions with an energy of 14.1 MeV by an anular source placed in the center of the tokamak's plasma volume.

4 Conclusions

A Geant4 program simulating the tritium breeding phenomenon inside a model tokamak has been designed. The geometrical model of the tokamak has been created and the physics has been added, by using the Geant4 tools and classes.

Four different breeding blanket designs have been implemented: a simplified WCLL (Water Cooled Lithium Lead) with pure PbLi, a HCPB (Helium Cooled Pebble Bed) with Li_4SiO_4, a HCPB with front beryllium neutron multiplier layer and a HCPB sandwiched between two beryllium layers.
Some simulations, each with 50000 input neutrons, have been performed and some results have been analysed. The Tritium Breeding Ratio (TBR) showed to increase in all designs as the ^{6}Li enrichment increases, as expected. All the HCPB designs showed TBR <1 with natural lithium (7.5.% ^{6}Li enrichment). The Be layers proved to increase the TBR in the HCPB design, however no particular difference has been observed between the HCPB with one Be layer and the HCPB with two Be layers. To conclude, the simplified WCLL (pure PbLi) showed the highest TBR.

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