

Thorium Nuclear Reactors: Spallation Target Optimization

Using Geant4 and Fluka

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Abstract

Thorium nuclear generation is one of the most promising fourth generation nuclear technologies. In these generators, uranium enrichment can be replaced by an accelerator driven system (ADS). An ADS is composed of a particle accelerator, a spallation target and a sub-critical core. This research is focused on the optimization of the spallation target, especially its length, in order to maximize the availability of neutrons to the thorium sub-critical core. The advantage of this approach is that it includes the target in the overall optimization process.

The research has been carried on in two phases. In the first stage, using G4beamline, I built a simulator that emulates a variable length target and then ran smaller scale experiments for both lead and thorium targets. The target length was optimized for maximum yield of fertile neutrons. In the second stage, I used FLUKA to run large scale simulations on identical geometries using lead targets only. In the FLUKA experiments, the target length was optimized for maximum neutron fluence and target radius was determined from neutron balance densities.

Findings were consistent across experiments and showed that the design of an ADS should include a target optimization for the desired energy and target material. Output sensitivity to target length is especially high for thorium targets. The range of lengths used in most research and pilot projects overlaps broadly with the range of optimality resulting from the experiments presented here. However, this work indicates that using a 300 mm or 600 mm target indiscriminately is suboptimal and can impact the efficiency of the thorium reactor.

1. Introduction

Countries and governments around the world need to meet electricity demand as fossil fuel sources are depleted and their price increases. Research of new technologies or the development of existing ones into commercial viability is needed. Both nuclear and renewable energy technologies are potential avenues, with advantages and disadvantages. What is common, though, is that both need funding and sustained research for the development of scalable, cost-effective solutions. The nuclear avenue in particular makes a reliable source of power. However, there are a number of serious problems with the existing (conventional) nuclear plants. New nuclear technologies, commonly referred to as fourth generation nuclear reactors, can solve these problems. Among these, molten salt reactors (MSRs) are one of the most promising.

An MSR is derived from the idea of a fluid-fueled reactor, which has been well researched since the start of the nuclear era. MSRs can accept various fluid fuels, the most typical being thorium. This is why the technology is commonly known as thorium nuclear generation. A simplified diagram of the energy production using thorium reactors is depicted in figure 1.

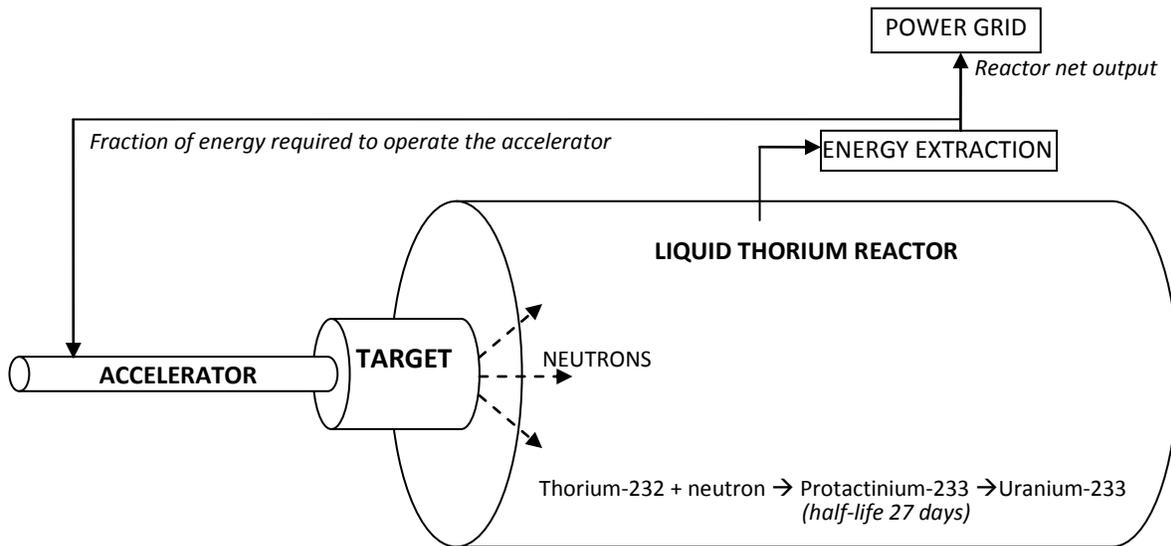


Figure 1. Diagram of an accelerator driven system (ADS) using a thorium reactor.

One of the major differences between a conventional reactor and an MSR is that the latter can use an accelerator to produce extra neutrons instead of uranium enrichment. An MSR that uses an accelerator forms an accelerator driven system (ADS). An ADS has three components: a proton accelerator, a heavy-metal spallation target, and a sub-critical core (the thorium reactor). The target acts as a neutron source

when struck by the beam and is neutronically coupled to the core [1]. The target can be placed in front or inside of the fluid-fueled reactor. An interesting feature of these reactors is that they can also use conventional reactor waste as fuel. Raja gives a good introduction to the physics of the fluid reactor [1]. Ait Abderrahim et al. [2] is a seminal work on accelerator driven systems.

Despite its venerable age, the MSR technology is still not mature and no large scale, economically viable power generator has been implemented yet. The Fukushima disaster sparked more interest in the research and development of MSRs around the globe, with countries like Norway and, most notably, India (India's Kakrapar-1 nuclear power plant has been using thorium instead of uranium for some years) expanding their current programs. New advances on the accelerator side of the technology are also making the system more efficient. Early research was focused on high energy accelerators [3]. However, promising results have been more recently obtained with lower energy accelerators [4, 5]. Diminishing the fraction of energy required to operate the accelerator is impactful, as it increases the reactor's net energy output (fig. 1) and also increases its reliability. Also, various target materials have been tested, and lead-bismuth eutectic has emerged as the preferred material for targets [6].

This research focuses on lower energy accelerators (0.5 GeV to 3 GeV range). High energy protons require, besides larger accelerators, big targets. Also, my experimental work will be centered on ADS with pure lead targets, as well as thorium ones. Both types have been less researched. Thorium would be a convenient target material from an operational point of view. Pure lead represents a fundamentally more efficient target material than lead-bismuth. The main drawback is that a lead target requires the reactor to function at higher temperatures compared to lead-bismuth ones, and this poses some technological challenges. Nevertheless, encouraging results for higher temperature thorium reactors have started to gain momentum [6, 7, 8].

Up to my knowledge, most of the existing research tries to maximize the number of neutrons produced per proton by varying the material of the target or the energy of the protons, i.e. beam energy ([2] gives an overview). However, little systematic research was done in optimizing the target dimensions. This is an interesting part of the technology because changing the target dimensions not only causes a difference in neutrons available for fission, but also modifies the costs related to the target itself. The paper addresses the optimization of the spallation target. In the first phase of the research, I used the Geant4 simulation engine to optimize the length of the spallation target. In the second phase, I built a new simulator with FLUKA, which uses a different engine and models hadronic interactions that are closer to industrial scale. Both length and radius were considered in this phase.

The paper is organized as follows: before starting the presentation of the method and optimization tools, a brief analysis of the advantages of thorium-based reactors relative to conventional ones is presented. This analysis is important to the research because it underlines the significant potential for

economic benefits of the technology. It also represents a huge motivation for the author to further the research and stay actively involved for the long term in multiple ways in the advancement of the technology. The results of the experiments from both phases are presented. They are followed by discussion, conclusions, and a future work roadmap.

2. Analysis of the advantages and disadvantages of thorium-based reactors

As with any nuclear method for energy generation, the advantages and disadvantages of thorium reactors can be analyzed on several dimensions.

Safety

Because MSR's do not use enriched uranium, they are subcritical, meaning that they constantly require some input of energy to burn their fuel. Thus, they are inherently safe: if one were to have a power failure at an MSR, the reactor would automatically shut down and dump its contents. In fact, scientists working on experiments such as Oak Ridge National Laboratory's Molten Salt Reactor Experiment (MSRE) regularly shut down the reactor by cutting power to it [9]. The other great difference is the state of the fuel. An MSR uses solely liquid fuel at atmospheric pressure, while conventional reactors use solid uranium pellets, usually in a pressurized chamber. The advantage of a liquid fuel is that it can easily be replaced and separated from neutron poisons (elements that absorb many neutrons) that naturally develop during fission; the poisons can then be removed from the reactor.

Thorium is also barely radioactive—the potassium in a banana emits more radiation than a sample of thorium of a similar mass. It is additionally an alpha particle emitter, the safest form of radiation; alpha particles usually cannot penetrate human skin [10].

On another safety dimension, the technology has the advantage that it substantially limits the potential for spreading weapon-grade nuclear material [11].

Mining

Thorium is 4-5 times more abundant on earth than uranium and can be mined much more easily [1]. It is also found with other rare earth elements, which are currently mined for a variety of uses. Because of its low radiotoxicity, it will not need heavily reinforced modes of transportation from the mining and processing site to the power plant.

Environmental Issues

Apart from thorium's low radiation, it is also fertile in its natural state, meaning that it does not have to be enriched in order to be able to be used in a reactor. The consequence is that each kilogram of mined thorium can be placed in the reactor, as opposed to only 14% of mined uranium [12]. MSR's can also burn many of the fission products that currently must be painstakingly removed from a conventional

nuclear reactor and subsequently placed in geological storage for centuries. Molten salt reactors can even use these fission products as fuel, not only ridding the world of environmentally dangerous long term storage and short term dry casks, but also creating energy with them [13]. The only serious byproduct of MSRs is a small amount of plutonium, which is needed for other applications, such as powering space probes [14].

Required Capital Investment

Because thorium reactors are inherently safe, they do not need to be as isolated from the densely populated areas as their conventional counterparts; they do not need triple redundancy in their safety systems or large exclusion zones. This greatly decreases start-up costs. And, with decreased capital costs, more reactors can be produced. Companies also do not need to pay as much for transportation of fuels, products and resulting energy.

Political will

Because it solves a number of critical issues that conventional reactors pose, thorium reactors are expected to be less controversial and easier to gain political backing. In this post-Fukushima world, where major countries decided to stop their nuclear programs, this technology can revitalize a nuclear future.

Scalability

Various forms of liquid reactors have existed in experimental phase for over 40 years. MSRE was one of the most successful nuclear experiments of the 60's. Scientists collected thousands of hours of data ([15] is a representative report). However, the test was never meant for economically viable energy generation because the methods available to create the additional neutrons required to achieve fission were not efficient. Unfortunately, despite major advances made during the past 50 years, the technology is not yet robust enough for commercial implementation. Therefore, the challenge currently undertaken by the research community is to devise an economically viable solution based of these proven principles. Unfortunately, new approaches to old principles require funding and political commitment, which is currently a problem and represents the biggest drawback of the technology.

3. Methods and Results — Geant4 Simulations

3.1 Optimization Criterion

The goal of this phase is to determine the optimal length of the lead target. As opposed to most of the existing empirical research, which focuses on maximizing the number of *generated neutrons* per proton, my approach is to maximize the number of neutrons that are able to enter in the fertile zone, i.e. the thorium. These neutrons will be called *fertile neutrons*.

The advantage of this approach is that it includes the target in the overall optimization process. Generated neutrons that have high energy interact with the target's atoms, creating more neutrons. The larger the target, the more neutrons are generated. However, the target also slows down all neutrons. Therefore, if the target is too large, some will not have enough energy to escape and will remain trapped in the target. If the optimization attempts to maximize the number of neutrons that escape and reach the fertile zone, it will create efficiency across the combined accelerator and target system (figure 1).

3.2 Software used for the experiments

For the experimental part of phase 1, I built a simulator that allows various measurements at different target lengths. Its core contains a particle simulation engine. Additionally, for the mining and representation of data I used a data analyzer.

3.2.1 The simulator: G4beamline

The simulation software that I used to build the simulator is G4beamline v2.08, created by Muons, Inc. It is a particle-at-a-time simulation program that uses the Geant4 engine [16, 17] and is optimized for simulating beamlines [18]. It uses a proprietary syntax that allows the programmer to define the geometry of the system (the components and their positioning) as well as the environment variables [19].

The simulator needed for my research should contain a beam source and a target. Simulations should then be run for various target lengths. The problem with G4beamline is that it does not allow for easy data collection for multiple values of the geometries and/or environment variables. Also, it embeds no optimization algorithm. Given the huge amount of data resulting from each simulation there is no chance that a home-made optimizer can be of any help. The solution that I found to overcome this problem is to emulate variable target lengths inside G4beamline by using in each simulation the equivalent of a long, fixed target and inserting detectors made of the same material at equal distances. For the purpose of optimization, any detector can be the end of the target and the neutrons escaping it the fertile neutrons. One of the conceptual geometries, including nine detectors, is shown in figure 2. The

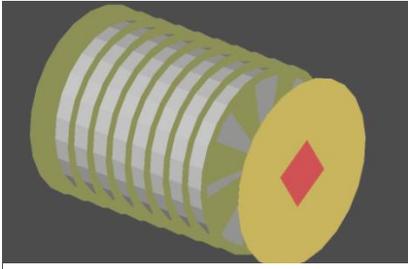


Figure 2. Conceptual geometry of the simulator used to emulate a variable length target. It contains the proton source (square), lead target (cylinder), and multiple evenly spaced detectors (circles).

components of the geometry are the proton source, shown as a square; the target, which is cylindrical; and the detectors used to obtain statistics about the neutrons. The neutrons that pass through a detector are fertile neutrons for that particular target length. The fertile zone is defined by the area of the detector.

The proton beam was generated at the center of the proton source. Its dimensions remained constant—it was a 10 proton Gaussian beam with standard deviation $\sigma=10$ micrometers (μm) and a maximum radius (such that there would be no chance of a proton generating outside of the proton source) of $100 \mu\text{m}$.

The energy of the beam was a controlled variable, ranging from 500 MeV to 3 GeV.

As explained above, the target also had constant dimensions, and was large enough to completely stop every neutron produced. It was cylindrical, with a radius of 3.5 meters and a depth of 3 meters. It started 50 mm from the proton source, and was made of lead for most of the experiments. In one comparative experiment, the target was also pure thorium.

Inseparable from the target were the detectors. I placed them at every 25 mm in the target, regardless of the experiment, with the maximum number of detectors used being 120. They were shaped as thin wafers, with radius of 3.5 meters. Because the Geant4 engine only allows particles to pass through one material at a time, the target had to be segmented 120 times. Each target segment had to be slightly shortened, and the detector was placed at the end of every one. Then, the target was pieced together to look as if it had no segments. The detectors did not interfere with the results since they were made from the same material as the target (lead or thorium). These detectors gathered data from each particle that passed through them: its energy, position, type (whether it was a neutron or not), momentum, etc.

3.2.2 The Analyzer: ROOT

The data analysis tool I used is ROOT v5.28, developed at CERN [20]. It is a tool developed by physicists for mining and representing the large amount of data that typically results from particle physics experiments. All plots and histograms from phase 1 were generated using ROOT.

3.3 Results

Using the 120-detector simulator that I built in G4beamline, I conducted three sets of experiments. Each set, which will be called for brevity an experiment, is composed of multiple simulations. Each simulation uses 100 runs with the same parameter set. The average of these runs is presented in a histogram. Figure 3 shows the visual output of a single run. It includes all generated particles (neutrons, muons, etc) and their trajectories. Protons cannot be seen on this scale. The target is in mesh visualization.

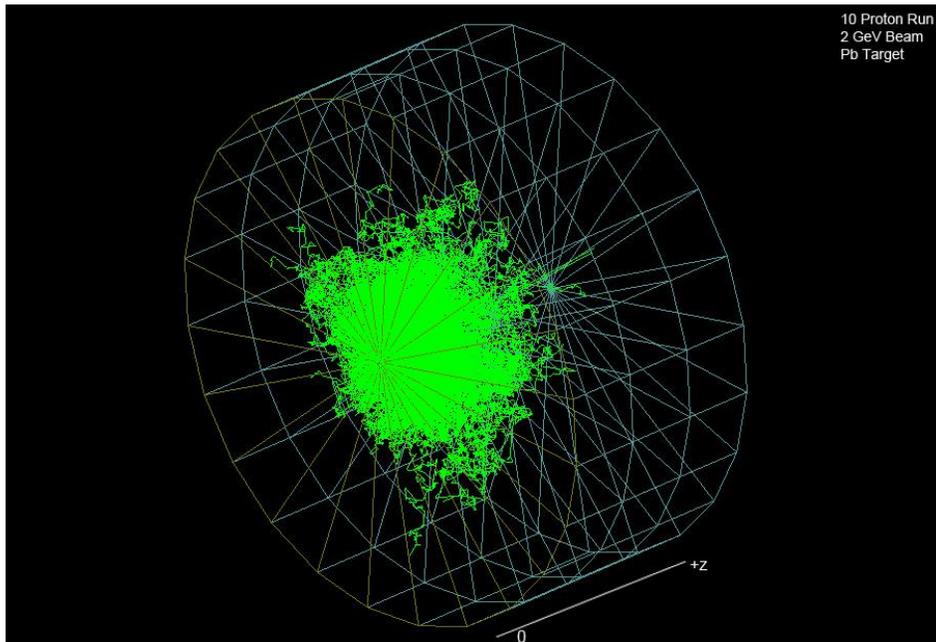


Figure 3. The visual output of a single run. Neutrons and their trajectories are plotted. Protons are oriented in the positive z direction, but are not visible on this scale. The target is in mesh visualization, where each section depicts one meter of the target with 40 detectors.

Geant4 Experiment 1

The goal of the experiment is to determine the length of the target where the neutron count is at a maximum (optimal length). Only the energy of the beam was varied. The range starts at 0.5 GeV and increases by 0.5 GeV until 3 GeV. The target material is pure lead. Results are presented in figure 4.

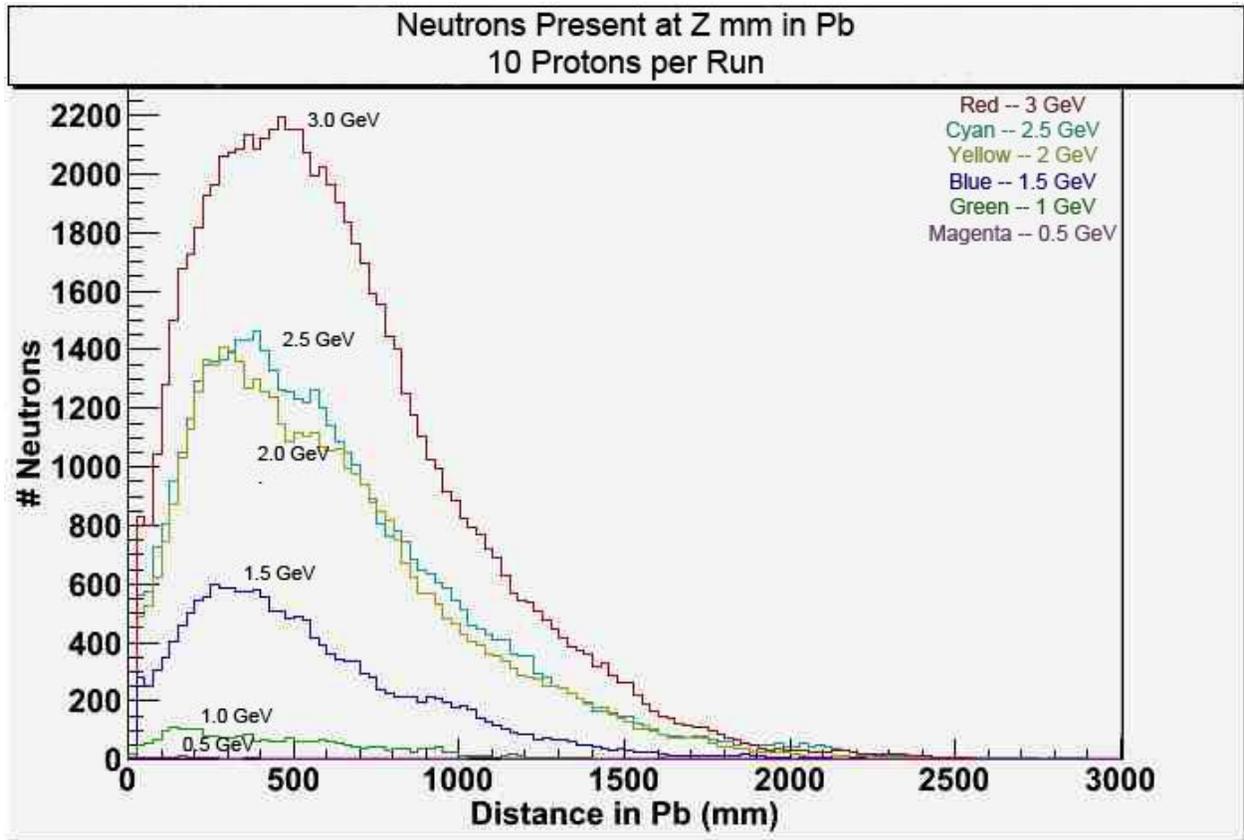


Figure 4. Plot of the results of experiment 1. It consists of six simulations at various beam energies, between 0.5 GeV and 3 GeV. Best target lengths depend on the energy of the protons.

Firstly, the results show that the optimal target length depends on the energy of the proton beam. Broadly, the higher the energy, the higher the length that ensures maximum production of fertile neutrons. Below 1.5 GeV there is no clear optimal length. The 1 GeV simulation shows only a weak optimum of 100-200 mm.

Secondly, the results help us evaluate the cost-benefit trade off in terms of beam energy. There is a clear benefit if one were to increase the energy from 1.5 GeV to 2 GeV. The fertile neutron count is raised by around 800, while the target length has to only be increased minimally. The marginal benefit of increasing the energy further, from 2 GeV to 3 GeV is significantly smaller. A similar increase in neutrons costs a 1 GeV increase, as opposed to 0.5 GeV, plus a longer target. The experiment shows that the greatest marginal benefit in the maximization of number of fertile neutrons occurs in the mid-energy range (1.5-2 GeV). The benefit of increasing the energy from 2 GeV to 2.5 GeV is surprisingly minor. Both energies were tested multiple times and the results were similar in each case. However, the asymmetry in neutron count compared to adjacent energies is hard to explain and requires further validation.

The optimal length for the 3 GeV beam is between 425 and 525 mm. For the preferred energy range (1.5-2 GeV) optimal lengths are: for 1.5 GeV 250-300 mm and for 2 GeV 275-350mm.

Geant4 Experiment 2

In this experiment, I focus mostly on mid-range energies that resulted as preferable for the lead target and do a direct comparison between a lead and a thorium target. Thorium would be the most convenient target material for the power plant operators, since they would not have to store extra fuel and target material separately. At each energy, there is a simulation for a lead target and a thorium one. Histograms for 1, 1.5, and 2 GeV energies are given in figure 5.

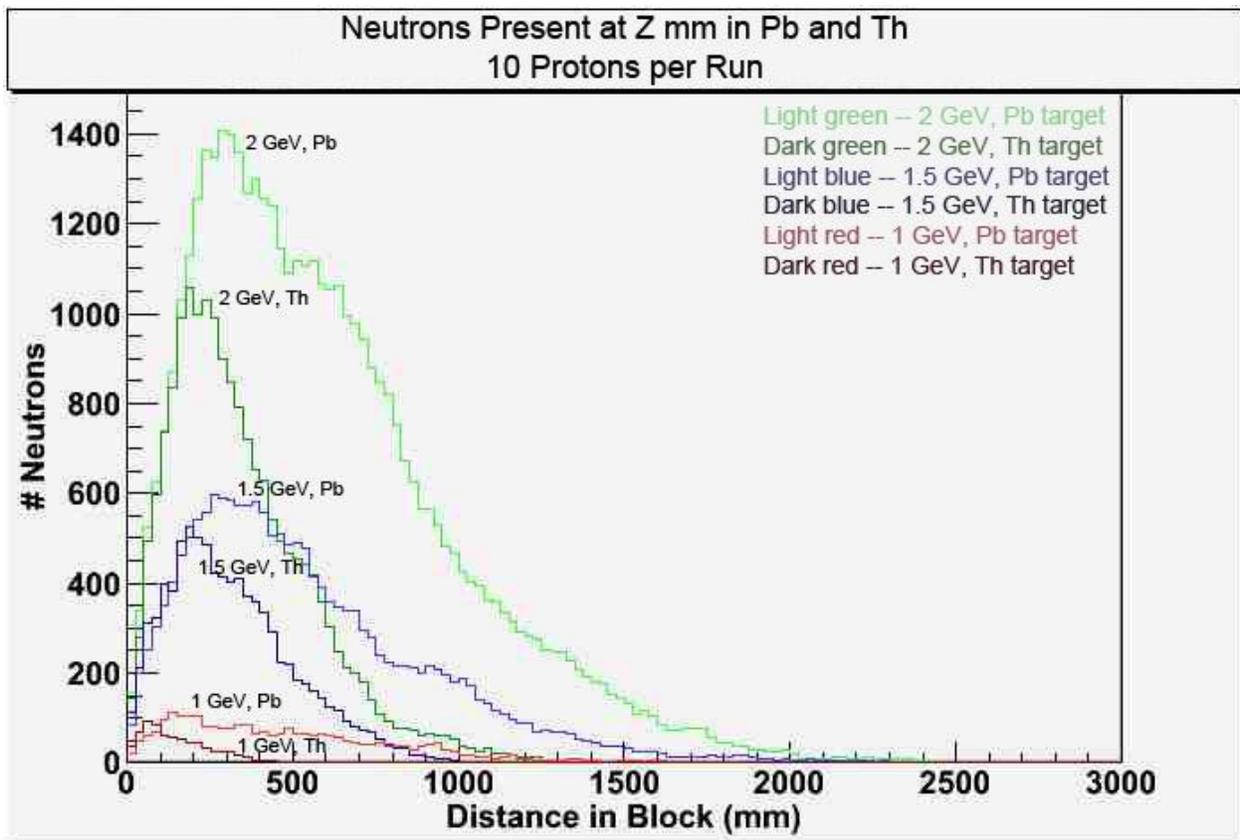


Figure 5. Plot of the results of experiment 2. 3 simulations at 1, 1.5, and 2 GeV per type of target. Two types of target: Lead and Thorium. The higher the energy, the better it is to use lead. Output sensitivity to target length is much higher at thorium.

As opposed to lead, which does not show a clear optimum at 1 GeV, the thorium target shows a 50-100 mm optimal length, which is an encouraging result (smaller targets not only are cheaper but also

allow for a smaller design of the reactor). Thorium target optimal lengths for the other energies are 175-250 mm for 1.5 GeV and 175-275 mm for 2 GeV.

The simulations show that at the lower energy (1 GeV) the thorium target seems a potential solution. Its yield of fertile neutrons is comparable to that of Pb. However, at the 1.5 and 2 GeV energies, which are also the preferred energies for lead, a lead target performs better: the higher the energy, the higher the marginal benefit of the lead target. However, the experiment also reveals several other interesting characteristics of the thorium targets.

Firstly, the output sensitivity to target length is much higher for thorium than for Pb. The number of fertile neutrons decreases significantly around the optimum for all energies. This suggests that a target optimization for thorium can potentially enhance the performance of the ADS even more than in the case of lead targets and has the potential of being a critical part of the design. Secondly, the experiment shows that one of the potential advantages of thorium as a target is that it might allow shorter optimal lengths, compared to lead. Thirdly, increasing the beam energy requires a smaller increase in the optimal length of a thorium target as opposed to one made of pure lead. The latter two characteristics could form a basis for interesting future research related to thorium targets.

Geant4 Experiment 3

The idea behind experiment 3 is to obtain a different type of measurement that would corroborate or weaken the results obtained at experiment 1. For this, I decided to look at proton energy as a function of the target length, believing that a correlation might be found in the position of the fertile neutron maximum and the amount of deposited proton energy. The energies used in the simulations are 1, 2, and 3 GeV. The results are presented in figure 6.

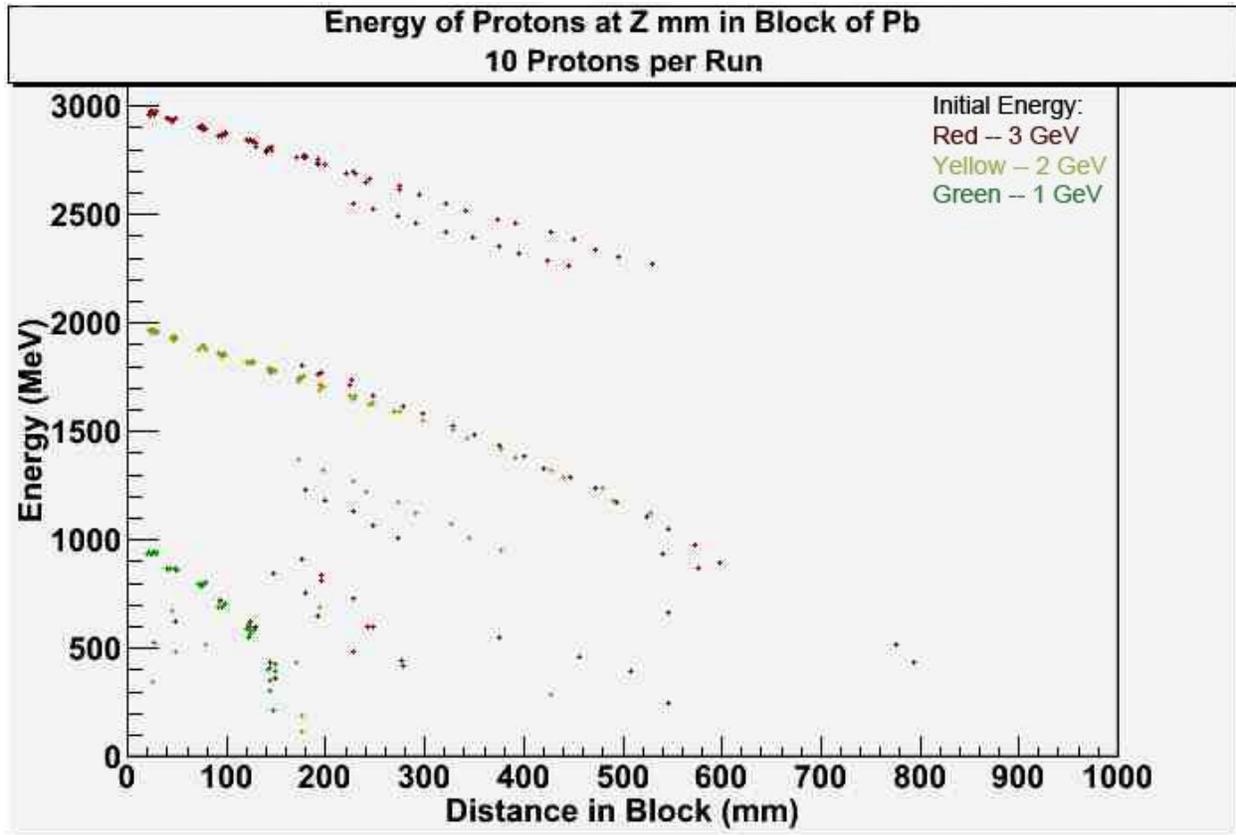


Figure 6. Plot of the results of experiment 3. The measured variable is proton energy in the lead target. Three simulations at 1, 2, and 3 GeV. Data shows that the length at which at least 90% of protons have already collided with the target atoms coincides with the optimal lengths for the same energies resulted in experiment 1.

The experiment indicates that at least 90% of protons have already collided with the target atoms at the following target lengths: for 1 GeV, 150 mm; for 2 GeV, 250mm; and for 3 GeV, 450 mm. The optimal lengths found in experiment 1 for these three energies were 100-200 mm for 1 GeV; 275-350 for 2 GeV; and 425-525 for 3 GeV. Therefore, the data corroborates the results in experiment 1. Additionally, the fact that the peak of the neutron count is where at least 90% of protons have already collided with target atoms indicates that protons have little, if any, impact after their first collision.

4. Methods and Results — FLUKA Simulations

4.1 Optimization Criterion

Given the well supported findings of the first phase, the decision has been taken to advance the research into a second stage. Using a more powerful simulator (FLUKA), I ran simulations on large numbers of primary particles (protons) in order to determine the optimal dimensions of the lead target.

In this stage, I used neutron fluence as the optimization criterion. Fluence (Φ) is a measure of the concentration of particle paths in an infinitesimal element of volume around a point in space [21]. If N represents the number of particles crossing a surface da perpendicular to the particle direction, $\Phi = dN/da$.

Given any surface S of infinitesimal thickness dl , if the angle between a particle direction and the normal to the surface is θ_i , the particle will travel a length $dl/\cos\theta_i$. Therefore, the average fluence through surface S is the sum of all paths per unit volume:

$$\Phi = \lim_{dl \rightarrow 0} \frac{\sum_{i=1}^N \frac{dl}{\cos\theta_i}}{Sdl}$$

and is measured in *particle/cm²*.

Fluence is a powerful measure for a number of reasons. On one hand, it is proportional to the density of collisions (the more distance traveled in a volume, the more interactions). Therefore, it is a good estimator of the interaction rate in a given volume. Thus, fluence is a way to measure particle density. On the other hand, fluence is independent of the incident angle of the particle beam. Neutron yield (number of particles crossing a plane per unit area) is the equivalent of planar particle fluence and does depend on the angle of incidence of the particle beam. In FLUKA, fluence is determined via a volume estimator as track length per unit volume per primary particle [21]. By multiplying by the total number of primaries, one can obtain the total particle track length per unit volume.

4.2 Software used for the experiments

4.2.1 The simulator: FLUKA

The simulation software is FLUKA v. 2011.2.x [22], a Monte-Carlo simulations package developed at CERN, and compiled with gcc/g77 (Fortran). It uses proprietary syntax to create the simulator. The FLUKA code started being developed in 1969 in Germany and at CERN, and has a long and interesting history [23]. Today it is one of the most powerful and widely used environments for hadronic simulations.

The geometry of the experiments is virtually identical to the one used in Geant4 for the specific reason of keeping as many parameters constant as possible across platforms. The beam could not be defined exactly as the Geant4 one; its Gaussian attributes had to be converted from σ to full width at half-maximum (FWHM). As the Gaussian function used has a normal distribution, the conversion could be simplified to $\text{FWHM} = 2\sqrt{2\ln 2} \sigma \approx 2.3548 \sigma$. The energy of the beam was still kept as a controlled variable. The target's dimensions and its distance from the beam source were the same as the ones in Geant4. FLUKA experiments were focused on lead targets.

The detectors, though, functioned differently than Geant4 ones. The FLUKA detector (USRBIN) scores distributions of several quantities in a regular spatial structure that is independent from the geometry. It is still a perfect detector—there is no error in its measurements and does not impede or alter particles in any way. However, instead of having many circular detectors, USRBIN is a cylindrical mesh that permeates the target, with R- Φ -Z bins; these bins have defined height, width, and length with respect to the cylindrical axis. As in Geant4, I defined 120 bins in the Z direction. The difference arises from the other binning qualities; the cylinder's radius is split into 175 bins (one bin for every two cm), and its circular cross-section (whose normal vectors are parallel to the Z axis) is split into 180 radial bins (one bin for every two degrees). The detectors scored two requested quantities—neutron fluence and neutron balance density.

4.2.2 The Analyzer: Flair

Flair [24] is an end-user interface closely linked to FLUKA. I used Flair v.0.9.2 to interface with FLUKA on all my experiments. It is based on Python and Tkinter and includes a FLUKA input editor; debugger, compiler and monitor for runs; a post-processor and plot generator interface through gnuplot; and other features.

4.3 Results

Using the FLUKA simulator I conducted three experiments. The first FLUKA experiment mirrors Experiment 1 from Geant4 (0.5-3 GeV proton beam, lead target) using this time 100,000 protons instead of 10 and neutron fluence as optimization criterion instead of neutron yield. A second FLUKA experiment is identical to the first, but runs with a 10 proton beam instead of 10^5 and aims to identify the effect of small sampling on the measurements. The last experiment deals with submerged lead targets and uses neutron balance density analysis to make a preliminary estimation of the optimal target radius.

FLUKA Experiment 1

As in Geant4, the goal of experiment 1 is to determine the optimal length of the target. There are two differences though. Firstly, the simulation is executed with 10^5 protons. Secondly, I measured the neutron fluence as opposed to neutron yield at various distances in the lead target. The simulations were done for the same beam energies. Results are presented in figure 7.

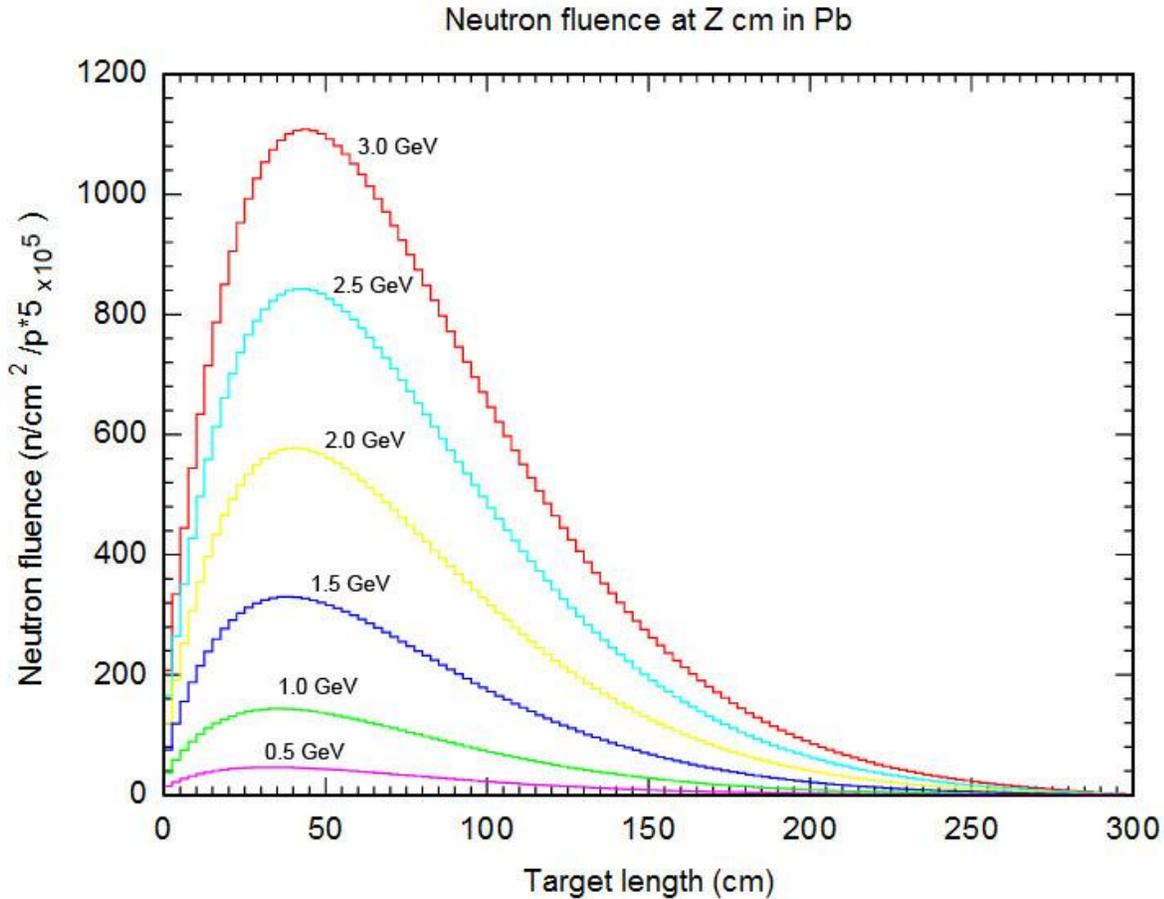


Figure 7. Plot of the results of FLUKA experiment 1. The measured variable is neutron fluence in the lead target normalized to the number of protons (total fluence). Six simulations, each with five cycles of 10^5 protons at various beam energies, between 0.5 GeV and 3 GeV. Similar to Geant4, optimal target lengths depend on the energy of the protons.

Similar to Geant4, the large scale FLUKA results show that the optimal target length depends upon the beam energy. Higher energies require longer optimal targets. Again, the 500 MeV and the 1 GeV have weak optima. The resulting optimal lengths are summarized in table 1, in the discussion section.

In terms of beam energy, simulations show again an absolute output benefit from increasing the energy. In percentages, the highest increases occur, as expected, at lower energies. For example, the percentage increase in total fluence from 1 to 1.5 GeV is more than 100%, while from 2.5 to 3 GeV it is around 30%. The FLUKA simulation does not confirm the asymmetry recorded with Geant4 for 2 and/or 2.5 GeV (fig. 4). Given the larger scale and the strength of the underlying models, it is likely that the FLUKA results are correct and the Geant4 outcome represents an anomaly.

FLUKA Experiment 2

This experiment reproduces the previous one, but only with 10 protons. The difference in the resulting optimal target length gives an indication of the effect of small sampling on the optimization. The results are depicted in figure 8 and numerical values for the target length are included in table 1 (discussion section). This experiment also allows a direct comparison with G4beamline results and helps to determine the impact of the new optimization criterion (fluence versus yield).

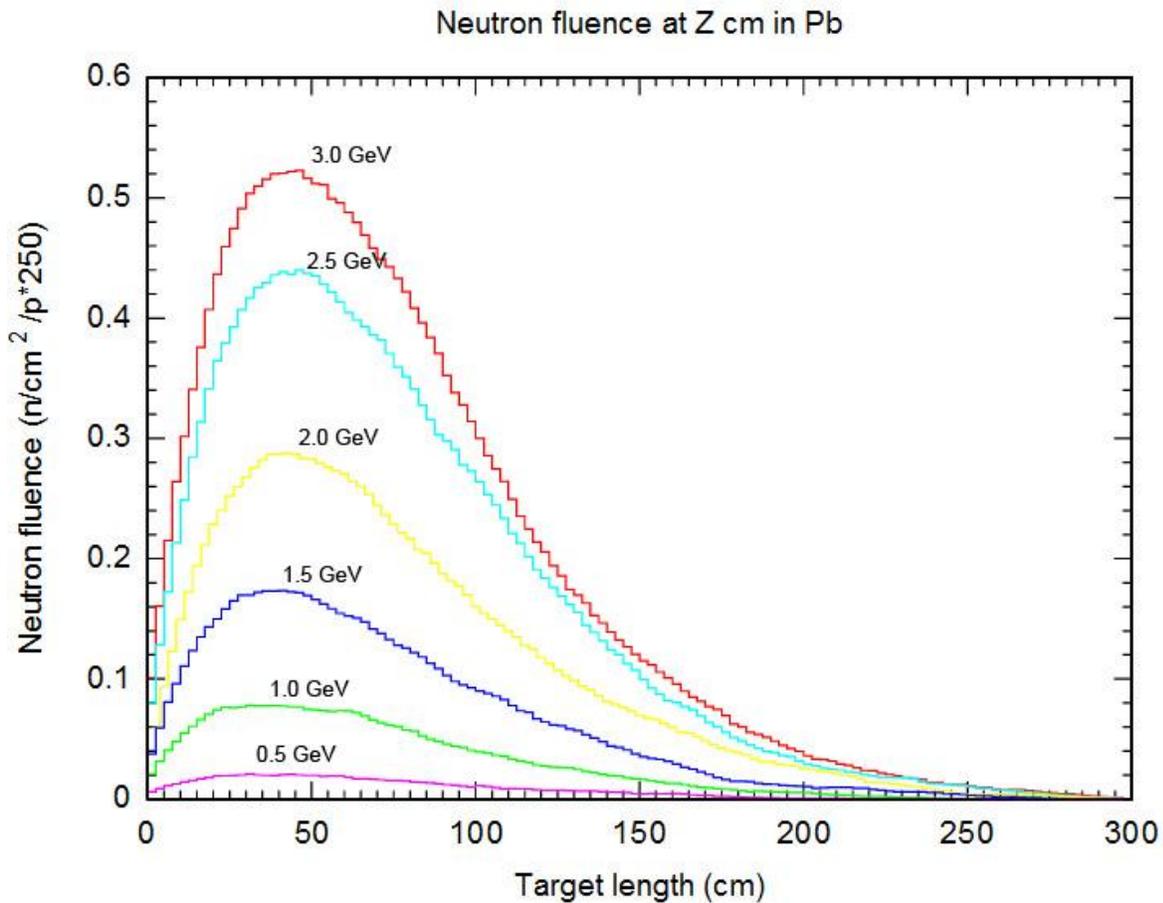


Figure 8. Plot of the results of FLUKA experiment 2. The measured variable is neutron fluence in the lead target normalized to the number of protons (total fluence). Six simulations, each with 25 cycles of 10 protons at various beam energies, between 0.5 GeV and 3 GeV.

FLUKA Experiment 3

So far, the experiments looked mostly at the neutron activity at the end cap of the target. Especially for targets placed inside the reactor, the optimization should consider maximization of neutron activity on the entire surface of the target, other than the entry cap. The third set of measurements analyzes the neutron balance density in order to make a first determination of radius. Neutron balance density is the algebraic sum of outgoing neutrons minus incoming neutrons for all interactions per unit volume per primary particle [22]. Figure 9 shows the progression of neutron balance density for increasing beam energies. Because it is plotted logarithmically, the balance is taken in absolute values.

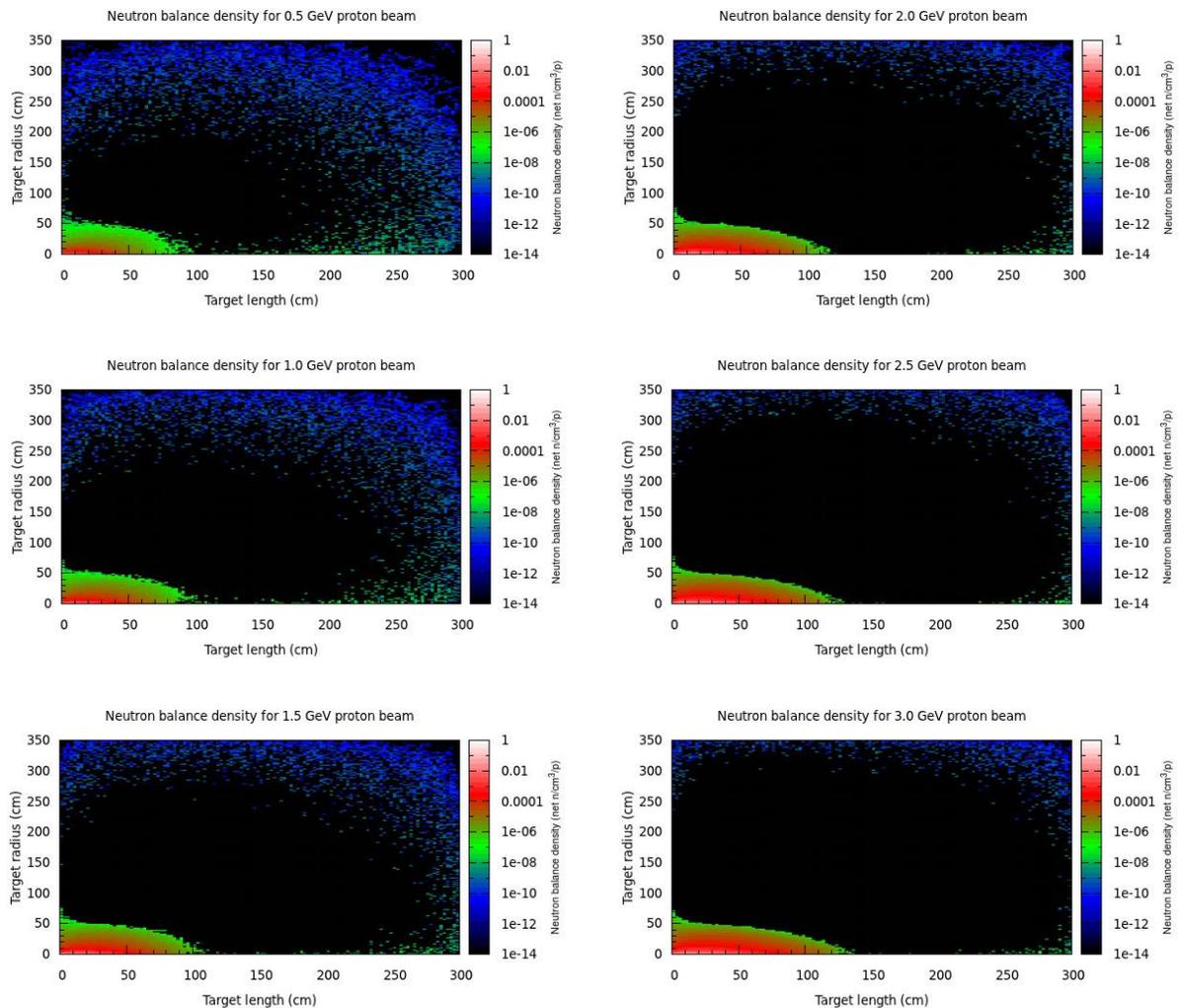


Figure 9. Plot of the results of FLUKA experiment 3. Neutron balance density is measured in the lead target at energies between 0.5 and 3 GeV. The plot presents the outcome of five cycles of 10^5 protons. The neutron-producing region is in all cases contained within a radius of about 50 cm. The neutral zone is wide (in black), but in most cases neutrons are absorbed at the periphery of the target.

The neutron producing area (bottom left) is followed by a large neutral zone, where there is no change in net neutrons (black area). After the neutral boundary, the absorbing region is visible as a halo. For low energy protons, the resultant neutrons are almost entirely absorbed by the large target. For each energy, most of the neutron producing area is contained within a 50 cm radius. The axial distribution though is much more sensitive to the proton energy and increases with it. However, there is little neutron production at lengths beyond 80 cm for 0.5 GeV, 85 cm for 1 GeV, 95 cm for 1.5 GeV, etc. This experiment indicates that both radius and length are important design parameters for the efficiency of the reactor. However, for a given target material, the radius could require less optimization for a specific energy while length shows high sensitivity to differences in primary particle energy.

5. Discussion of Results

The main results of both Geant4 and FLUKA experiments are summarized in table 1.

Table 1. Summary of experimental results for the optimization of the target length

Beam energy	Optimal target length (Pb target)		
	FLUKA 10 ⁵ proton	FLUKA 10 proton	G4Beamline 10 proton
[GeV]	[cm]		
0.5	28-37	weak optimum	weak optimum
1	35 - 37.5	30-40 (weak)	10–20 (weak)
1.5	35-40	35-42.5	25–30
2	37.5-42.5	35-45	27.5–35
2.5	40-45	40-45	38-42
3	42.5–47.5	42.5-47.5	42.5–52.5

Compared to G4beamline, the large scale FLUKA simulations led to longer optimal targets: the lower the energy, the bigger the difference. The only exception is the 3 GeV optimization, where a 42.5cm lead target resulted as optimal across all simulators. The inherent differences in the hadronic physics models are not big enough to explain these changes. In my view, there are two major reasons that are likely to explain the difference.

One reason is that, at the lowest energies, the Geant4 neutronic statistics are quite imprecise as the number of neutrons produced by the 10 primaries is very low. The 10-proton FLUKA simulation (Experiment 2) helps to evaluate the effect of small sample. In this experiment, at 1 GeV the maximum fluence was recorded at smaller lengths compared to the full scale simulation, although the exact same simulator was used. Overall though, even for lower energies, the small sampling seems to affect mostly the quality of the result (wider, more uncertain optima) than the actual value of the optimal length. Moreover, for higher energies, it has no effect, the same optimal lengths being obtained using small scale and large scale simulations with the same simulator.

The second, probably more relevant cause of the differences in optimal lengths between Geant4 and FLUKA results is the angular distribution of the neutrons. The higher FLUKA values for the target length indicate that fluence continues to increase for a few centimeters after the neutron yield peaks. This effect is very important at lower energies (for example, small scale fluence-based optimum is at least 10 cm longer at 1GeV compared to the yield-based one) and diminishes with the increase of incident energy. This is explained by the fact that the particle distribution is much more radial around the area of maximum generation at lower energies. At higher energies, the distribution in the area of maximum generation is considerably more axial; therefore, the path lengths are closer to the normal path lengths and, consequently, fluence is closer in value to the neutron count. Given that fluence is independent of the angular distribution, there is benefit in using it for optimization, especially for lower energies.

It is interesting to note that for the studied energy range, in FLUKA calculations, the relationship between the optimal length - determined by maximizing the neutron fluence - and the beam energy is linear and follows approximately the relation $Z_{opt[cm]} = 30 + 5E_{Beam[GeV]}$. Based on these measurements, each extra GeV of incident proton energy requires 5 more centimeters of lead target.

6. Conclusions and Future Work

In my view, the most important finding, consistent across all simulations, is that at different beam energies, optimal target lengths are different. This indicates that the design of an ADS should include a careful optimization of the target for the desired energy and specific target material. For lead targets and energies below 1 GeV, this seems less critical as there is no pronounced maximum for the output. However, at higher energies, there are distinct optimal lengths.

Up to my knowledge, most research and pilot thorium energy generators consider target lengths as an input for the research and/or design. Common lengths span a range between 30 cm and 60 cm, the most typical being 60 cm [25]. The range that resulted from my experiments (35-42.5 cm for 1-3 GeV) is similar. However, important differences in performance occur at different energies. This experimental

work indicates that using a 60 cm target indiscriminately is likely suboptimal and will impact the efficiency of the thorium plant. At higher energies, the suboptimality is more costly, as the peak of both fluence and neutron yield is more pronounced.

Although it was not the main focus of this work, a thorium target appears to be a practical solution for low energies; it shows a considerable output sensitivity to target length and requires a smaller length. In my view, these findings should encourage future research for this material, which is convenient for the plant operator and, to my knowledge, has not been researched extensively.

The next stage of this research is to build a simulator that will allow for the systematic optimization for the neutron fluence and/or yield measured on the entire surface of the target, with the exception of the entry cap. The two-variable optimization (length-radius) likely requires modification within the FLUKA code itself, but it will allow a thorough investigation of the optimal dimensions for targets placed inside the reactor. The first step will involve regular target shapes (e.g. cylindrical) but further down the road the parabolic profiles suggested by the neutron balance density shape might be considered. Simultaneously, extending the simulations to a wider range of materials can help to find the best target material and dimensions for a specific set of requirements (e.g. beam energy, reactor size, etc). Additionally, improving the optimization criteria, for example by using both fluence and energy spectra can further improve the efficiency of the system.

References

- [1] R.Raja, *Accelerator Driven Nuclear Energy - The Thorium Option*, Fermilab Colloquium, 18 March 2009, Batavia (USA).
- [2] H. Ait Abderrahim *et al.*, *Accelerator and Target Technology for Accelerator Driven Transmutation and Energy Production*, DOE White Paper on Technology for Accelerator Driven Systems. September 2010.
- [3] R.R. Wilson, *Very big accelerators as energy producers*, Fermilab Report FN-0298, Batavia (USA), 9 August 1976.
- [4] S. Chigrinov *et al.*, *Nuclear Data Evaluation and Experimental Research of Accelerator Driven Systems Using a Subcritical Assembly Driven by a Neutron Generator*, Thorium Fuel Utilization: Options and Trends - Proceedings of Three IAEA Meetings Held in Vienna in 1997,1998 and 1999, International Atomic Energy Agency, Vienna (Austria), 2002, p. 207.
- [5] T.Y. Eom, J.B. Do, Y.D. Choi, K.K. Park, I.K. Choi, *Thorium Fuel Cycle Concept for Kaeri's Accelerator Driven System Project*, Thorium Fuel Utilization: Options and Trends - Proceedings of Three IAEA Meetings Held in Vienna in 1997,1998 and 1999, International Atomic Energy Agency, Vienna (Austria), 2002, p. 54.
- [6] OECD Nuclear Energy Agency, *Accelerator-driven Systems (ADS) and Fast Reactors (FR) in Advanced Nuclear Fuel Cycles. A Comparative Study*, Paris (France), 2002.
- [7] J.J. Park, D.P. Butt, C.A. Beard, *Review of Liquid Metal Corrosion Issues for Potential Containment Materials for Liquid Lead and Lead-bismuth Eutectic Spallation Targets as a Neutron Source*, Nuclear Engineering and Design, vol. 196, no. 3, 315-325, 2000.
- [8] G. Bauer, M. Salvatores, G. Heusener, *The MEGAPIE Initiative – Executive Outline and Status as per November 1999*, Paul Scherrer Institut, Villigen (Switzerland), 1999.
- [9] S. E. Beall, P. N. Haubenreich, R. B. Lindauer, J. R. Tallackson, *MSRE Design and Operations Report, PART V: Reactor Safety Analysis Report*, Oak Ridge National Laboratory Report TM-732, Oak Ridge (USA), August 1964.
- [10] J. Kennedy, J. Kutsch, *U.S. Heavy Rare Earth Cooperative. Global Economics of Thorium Energy*, Presentation at the 3rd Thorium Energy Alliance Conference, Washington (USA), May 2011.
- [11] A. Siddiqui, S. Fleten, *How to Proceed with the Thorium Nuclear Technology: a Real Options Analysis*, Energy Economics, vol. 32, no. 4, 817-830, July 2010.

- [12] R. Hargraves, R. Moir, *Liquid Fluoride Thorium Reactors: An old idea in nuclear power gets reexamined*, American Scientist, vol. 98, no. 4, 304, July 2010.
- [13] Y. Kadi, J.P. Revol, *Design of an Accelerator-Driven System for the Destruction of Nuclear Waste*, Workshop on Hybrid Nuclear Systems for Energy Production, Utilisation of Actinides & Transmutation of Long-Lived Radioactive Waste, Trieste (Italy), 3 - 7 September 2001.
- [14] K. Sorensen, K. Dorius, *Introduction to FlibeEnergy*, Presentation at the 3rd Thorium Energy Alliance Conference, Washington (USA), May 2011.
- [15] R. B. Briggs, *Molten - Salt Reactor Program Semiannual Progress Report for Period Ending August 31, 1965*, Oak Ridge National Laboratory Report ORNL - 3872, Oak Ridge (USA), December 1965.
- [16] S. Agostinelli *et al.*, *Geant4—a simulation toolkit*, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 506, no. 3, 250-303, July 2003.
- [17] J. Allison *et al.*, *Geant4 developments and applications*, IEEE Trans. on Nuclear Science, vol. 53, no.1, 270-278, Feb 2006.
- [18] G4Beamline - Particle Tracking in Matter-Dominated Beam Lines, <http://www.muonsinc.com/tiki-index.php?page=G4beamline>
- [19] CERN, Geant4 - a toolkit for the simulation of the passage of particles through matter, <http://geant4.web.cern.ch/geant4/>
- [20] CERN, ROOT - A Data Analysis Framework, <http://root.cern.ch/drupal/>
- [21] CERN, *FLUKA Estimators and Scoring*, 6th FLUKA Course, CERN, 23-27 June 2008.
- [22] CERN & INFN, The Official FLUKA Site, <http://www.fluka.org>
- [23] A. Fasso *et al.*, *The FLUKA Code: Present Applications and Future Developments*, Conference for Computing in High Energy and Nuclear Physics, La Jolla (USA), 24 - 28 March 2003.
- [24] CERN, Flair or FLUKA, <http://www.fluka.org/flair/index.html>
- [25] C. Bungau, R. Barlow, A. Bungau, R. Cywinski, *Neutron Spallation Studies for an Accelerator Driven Subcritical Reactor*, Proc. of the 23rd Particle Accelerator Conference 4 – 8 May 2009, Vancouver (Canada), p. 1351.