Faculty of Applied Physics

New Filter Design with Monte Carlo Calculation

BSc. Thesis

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Summary

Boron Neutron Capture Therapy (BNCT) is a very promising treatment for patients suffering gliobastoma multiforme. Although the first clinical trials on BNCT dates to the 1950s, BNCT research is still in phase I/II, i.e. the research is still being focused on the effects of the treatment on healthy tissue and treating the disease. According to the research of V.A. Nievaart[1], these two phases of the research, the spectral tailoring for BNCT, consists of two parts:

1. Defining the source neutron energies of the BNCT treatment beam in order to obtain the most ^{10}B absorption reactions in the tumor. In addition, the location, direction and dimensions of the BNCT treatment need to be optimized for every individual tumor size and location.
2. Developing and constructing the filter with the appropriate materials and obtain the right neutron spectrum for irradiation.

This thesis deals with the second part of the spectral tailoring, where was tried to write a program that can optimize the thicknesses of materials in the filter taking the neutron spectrum of the radiation beam into account. For the wanted neutron spectrum the relevant conclusions of the PhD thesis of V.A. Nievaart were used. He stated that having three neutron beams, one nearly thermal (5 eV) and two epithermal (500 eV and 10 keV), assures an optimal treatment. This was taken into account to define a proper goal function. Since the neutron current is a function of the thickness of the materials, the goal function is also a function of thickness.

In many literature the following definitions could be found for *thermal*, *epithermal* and *fast* neutron energy regions. Neutrons having energies below 0.5 eV are called *thermal*, between 0.5 eV and 10 keV are *epithermal* and above 10 keV and below 20 MeV are called *fast*. Since the goal function used to optimize the filter/ moderator arrangement is simply the *thermal* neutron current divided by the total neutron current, I have made a slight change to that definition. I call neutrons having energies below 5 eV *thermal*, between 5 eV and 10 keV *epithermal* and above 10 keV and below 20 MeV *fast*, so that the optimal spectrum Nievaart concluded in his thesis are all *epithermal* neutrons. Another criterion that must be satisfied during the optimization is that the *epithermal* neutron current should not be less than 1 per cent of the number of 'source' neutrons.

The simulation of neutrons traveling through materials was done by use of Monte Carlo calculations. With this program the shape of the filter/ moderator arrangement was defined and the neutron source and tallies were introduced. To read the Monte Carlo output file and write a new input file for optimizing the filter/ moderator arrangement an optimization script was written in Perl.

For *N-1* materials, the optimization script has the following shape:

[1] He did research to the spectral tailoring of BNCT at the Delft University of Technology within a cooperation of the Institute for Energy of the Joint Research Centre (JRC) of the European Commission in order to obtain its doctor degree.

```
Some parameters

While (precision > certain number) {

        MCNP input file

        For (i = 1 to N) {
          if (i = 1) {determine gradient material 1}
          if (i = 2) {determine gradient material 2}

          if (i = N-1) {determine gradient material N-1}
          if (i = N){determine precision = sum of all
            absolute values of the gradients}
          }

Save all relevant data

}

Run finished! You can have coffee now!
```

The optimization method used in the optimization script was the gradient ascent method. This method is based on the principle that any at least one differentiable real-valued function $F(\mathbf{x})$ increases most in the positive direction of its gradient. The gradient was determined by measuring the discrete derivative for a certain thickness. This was done by measuring the goal function difference when the thickness increases by 5 per cent. In the gradient ascent method, the gradient has been scaled by a factor γ to tune the step size. In this thesis, one run is done with γ constant and one run with a variable γ. For the optimization I have presumed that a maximum in the goal function gives the best radiation beam.

The optimization was done by only varying the thickness of the materials, therefore the materials and numbers of materials should be chosen beforehand. To make a selection of materials which could be used to moderate the neutrons, their cross sections are investigated. Since the filter should not absorb the neutrons, the *absorption* cross section should be low for neutron energies higher the 5 eV (*epithermal).* The *thermal* neutron current must be minimized and therefore the *absorption* cross section should be high in the energy region lower than 5 eV (materials such as Li-6 or B-10 have such properties). Neutrons from the neutron source have an average energy of around 2 MeV, therefore the filter should have a high *scatter* cross section for at least the high energy range (materials such as aluminum, argon, carbon, silicon, etc.). To absorb γ-radiation materials with high mass numbers should be used (such as bismuth or lead), but since they are also good neutron absorbers, they can not be used without having influence on the quality and intensity of the irradiation beam.

For first practice, the goal function was measured for several thicknesses of carbon (0.1-80.1 cm with increments of 0.1cm), combined with 10 cm Al_2O_3 and 0.1 cm B-10. From this first practice it could be seen that the *epithermal* neutron current was still too low (less than 5% of the number of incoming neutrons). What also could be seen from this first practice is that when the total neutron population becomes too low, the uncertainty in measuring the

neutron population increases rapidly, therefore the number of neutrons tracked should increase if the neutrons detected decrease.

After this first practice the optimization script has been run. This script had the following input parameters: a mono-energetic neutron source with energy of 2 MeV; filter materials Al_2O_3 and C with a variable thickness and B-10 with a constant thickness of 0.1 cm. The neutrons were tallied in the three different energy regions defined earlier. The factor γ was taken constant and had a value of 50 and was chosen arbitrary. The optimal thickness for the Al_2O_3- and C layer are respectively 15.83 cm and 15.98 cm. The *epithermal* neutron current is 2.46e-2 with respect to the total source neutrons and the goal function has a value of 0.46.

The same filter/ moderator set up (FM set up), but with a variable gamma, defined as the inverse of the goal function, results in an optimal thickness for the Al_2O_3- and C layer of respectively 18.79 cm and 18.77 cm. The *epithermal* neutron current is 1.29e-2 and the goal function has a value of 0.54.

As a last run SiO_2, C and Li-6 has been tested as filter materials. The SiO_2- and C layer were taken variable and the Li-6 layer had a thickness of 1.5 cm. When the SiO_2- and C layer had both a start thickness of 15 cm, the precision was below 0.01, namely 0.00985. And when both thicknesses were 18 cm the precision was 0.0580. When SiO_2- and C layer had a start thickness of 10cm and 15 cm the precision was bigger than 0.01, though the run was terminated after 14 runs due to *runtpe*[2] files created in previous runs. Therefore a command line must be inserted in the optimization script to delete all unnecessary MCNP output, so that this will not happen again.

From this thesis the following suggestion can be made for proceeding research:

1. Define a better goal function, in which only the three neutron beams are taken into account that V.A. Nievaart concluded;
2. Use a better/ different optimization method, by inserting a command that varies the number of histories tracked in MCNP, in order to obtain more accurate results from an MCNP run;
3. Reduce computation time, by using variance reduction techniques in MCNP or neural networks to train the script or even learn the script from several MCNP outcomes so that MCNP isn't in fact necessary anymore;
4. Insert a more realistic neutron source.

[2] MCNP creates files in which information of the run has been stored. These files are not deleted automatically after each run and therefore one must do that by himself. If a *runtpe* already exists MCNP creates a *runtpf* file and so on.

1. An Introduction to Boron Neutron Capture Therapy

1.1. Introduction

This chapter will give a brief summary of the concepts of Boron Neutron Capture Therapy (BNCT). Paragraph 1.2 will provide the principal working of BNCT as also a short history and the current status of BNCT. Nowadays, the research to BNCT consists of two parts, which will be discussed briefly in paragraph 1.3. After that the neutron beam parameters and characteristics will be discussed as also which influence they have at the human tissue, therefore I refer to paragraph 1.4. Finally the scope of this thesis will be given in paragraph 1.5.

1.2. General introduction BNCT

1.2.1. Basics of BNCT

Boron Neutron Capture Therapy is based on the principle that two components kept separate have relatively minor effect on cells but that when brought together it results in cell destruction [4]. This provides a way to selectively destroy malignant cells and spare normal cells [3]. These components are ^{10}B and neutrons. ^{10}B is very useful since it has a very high capture cross section at thermal neutron energies[3], see Figure 1-1. When only the malignant cells contain ^{10}B and the tissue is irradiated with a neutron beam, the 'bad' tissue will be destroyed and the healthy tissue will remain in tact. This is given schematically in Figure 1-2.

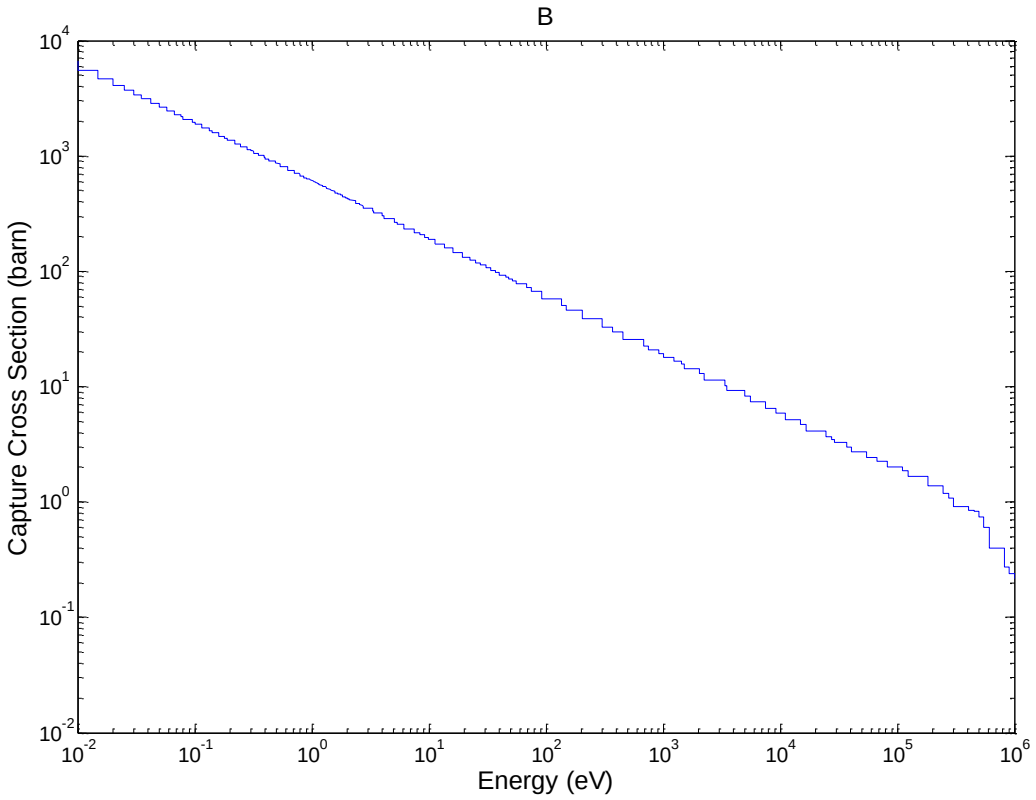

Figure 1-1 Capture cross section of B-10.

[3] Since the capture cross section is proportional with 1/E in the thermal region and since cross sections are related to probabilities of interaction with a certain material, the change of interaction is higher for lower neutron energies for ^{10}B (Further more details in section 2.2.1).

When ^{10}B captures a neutron a nuclear reaction takes place and releases an alpha particle and a lithium ion. This so-called (n,α) absorption reaction is schematically given by [3]:

$$^{10}B + {}^{1}_{0}n_{th}(0.025\ eV) \rightarrow \left[{}^{11}B\right] \rightarrow \begin{cases} {}^{7}Li + {}^{4}He + 0.48\ MeV + 2.31\ MeV\ (94\%) \\ {}^{7}Li + {}^{4}He + 2.79\ MeV\ (6\%) \end{cases} \quad (1.1)$$

Due to the fact that the reaction products (the alpha particle and lithium ion) travel a short distance in tissue (less then 10μm, which is similar to the size of a human cell [2]), there is a high probability that this reaction results in cell destruction and if only the tumor or 'bad' tissue contains ^{10}B (see Figure 1-2), only the 'bad' tissue is damaged.

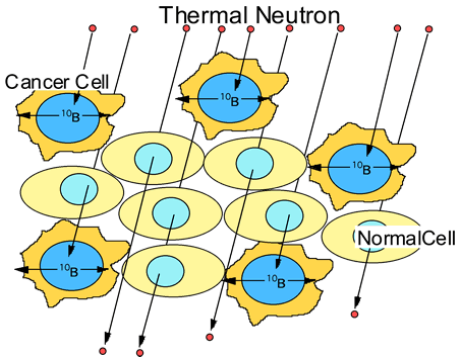

Figure 1-2. Schematic of irradiation of malignant or 'bad' cells containing a certain amount of ^{10}B. According to the reaction products of the (n,α) absorption reaction only the 'bad' cells will be destroyed.

The (n,α) absorption reaction is most efficient when the neutrons have energies below 0.5 eV, these neutrons are also indicated as *thermal* neutrons. Between 0.5 eV and 10 keV the neutrons are indicated as *epithermal* neutrons and *fast* neutrons have energies above 10 keV and below 20 MeV.

1.2.2. Brief history of BNCT

(This section will be a brief outline taken from [7]).
Fermi had discovered that this (n,α) absorption reaction is most efficient with a number of elements when the neutrons are slowed by passage through a hydrogen-rich substance. Later on Goldhaber et al. showed that when boron, lithium and nitrogen were irradiated with slow-neutrons, charged particle tracks were detected in photographic plates. The tracks from boron disintegration were short and straight. The (n,α) absorption reaction with boron is given by Eq. (1.1) and the two particles travel in opposite direction, with an average path length of approximately 7.6μm.

In 1936 Locher proposed to use this for radiation therapy. He pointed out that the first requirement, a source with an adequate neutron flux, would be difficult to achieve. But he did mention the medical usefulness, "the possibility of destroying or weakening the cancerous cells, by the general or selective absorption of neutrons by these cells". The injection of a soluble non-toxic compound containing boron, lithium, gadolinium or gold into bad tissue could be used for the radiation therapy.

Kruger and Golghaber began experiments with mouse tumors in 1938. They discovered that slow neutron dose to tumors containing H_3BO_3 were much lower to prevent tumor re-growth than were required for X-rays or fast neutrons.

The first trials on humans were done in the 1950s at the Brookhaven National Laboratory's. Ten patients were treated for gliobastoma, but the therapy was not successful, all patients died within 21 weeks, which was normal for gliobastoma patients treated by any means during the 1950s. Up to 1961 another 18 patients were treated, but all were unsuccessful and the BNCT project was halted in the US [2].

In 1968 Japanese researchers were more successful investigating new boron compounds. Up till now, more than 200 patients are treated in Japan of whom some survived for a long term [2]. Due to the success in Japan new BNCT trials were started in the US in 1994 and 1996. Also in 1997, a European trial at the High Flux Reactor (HFR) in Petten (NL) started under medical supervision of the university hospitals in Amsterdam (NL) and Essen (D) [2].

1.2.3. Current status of BNCT

Although the research to the concept of BNCT is going on for more than fifty years, all the current work is still under investigation [1] or, according to the thesis of V.A. Nievaart [2], only phase I/II[4] of clinical trials are performed with only a relatively low number of patients involved. The two major challenges the BNCT researchers are faced with are: i) Finding a proper ^{10}B carrier which brings the ^{10}B only to the malignant tissue and stays out of the healthy tissue, since that will cause destruction of healthy tissue and ii) designing a treatment beam which brings neutron with the right energies at the right location while minimizing the dose to healthy tissue.

This latter issue, about finding the optimal source neutron energies and direction is studied by V.A. Nievaart [2]. He concludes that in BNCT besides the 10 keV epithermal source neutrons, low epithermal source neutrons of around 1 eV and thermal source neutrons with energies of 0.1 eV must also be used. His work shows that significant improvements in the delivery of a therapeutic radiation dose can be given if a new neutron filter is designed in order to provide a variable neutron spectrum.

1.3. Spectral tailoring

Several articles can be found about the selection of the proper neutron spectrum, see for example [4-6]. About finding the right neutron energy spectrum these articles focus on the application of filter and moderator materials, the shape of the neutron beam and the quality of the resulting beam. Actually, according to V.A. Nievaart [2], the spectral tailoring for BNCT consists of two parts:

1. Defining the source neutron energies of the BNCT treatment beam in order to obtain the most ^{10}B absorption reactions in the tumor. In addition, the location, direction and dimensions of the BNCT treatment need to be optimized for every individual tumor size and location.

[4] There are four different phases for clinical studies. Studying the effects of the treatment on healthy tissue (phase I), after which the focussing is shifting towards treating the disease (phase II) and come to a scheme to treat the disease optimally (phase III) and ends with registering the treatment (phase IV).

2. Developing and constructing the filter with the appropriate materials and obtain the right neutron spectrum for irradiation.

The second part is the main issue of this thesis.

1.4. Desired neutron beam quality

(This section will be a brief outline taken from section 1 by IAEA [1]).
To optimize the filter/ moderator system there are two principal beam characteristics of interest, i.e. the beam intensity and quality. In the first section, the intensity will be discussed, where in the second section the quality of the neutron beam will be highlighted. In Table 1-2 beam characteristics and the power of five reactors are given.

1.4.1. Epithermal beam intensity

The desired minimum beam intensity would be 10^9 epithermal neutrons $cm^{-2}s^{-1}$. Lower intensities could be used, but will result in longer irradiation times, which is unappreciable. Higher intensities could shorten the irradiation time, but there is a chance that the quality would decrease. Most practitioners would rather have better quality rather than more intensity, within the constraint of having a reasonable treatment time (approximately one hour).

The tumor boron concentration will affect the requirements of the beam intensity. If the boron concentration would be greater, the intensity or treatment time could decrease. On the other hand, if the beam intensity is too low, it would be difficult to maintain the necessary boron concentration in the tumor during the irradiation time.

1.4.2. Beam quality

I. Fast neutron contamination

The fast neutron component is taken from energies higher than 10 keV. Fast neutrons produce high LET (linear energy transfer) protons (see Table 1-1), therefore one of the main objectives for BNCT beam design is to reduce the fast neutron component of the incident beam as much as possible. A target number should be $2x10^{-13}$ Gy cm^2 per epithermal neutron.

II. Gamma contamination

Since there are also (n,γ) reactions taking place inside the patient, the gamma contamination should be reduced as much as possible. This should also be considered in choosing the right materials for the filter, since there could also (n,γ) reactions taking place. Nevertheless, a target number should be $2x10^{-13}$ Gy cm^2 per epithermal neutron.

III. Ratio between thermal and epithermal neutron flux

Thermal neutrons will give a high dose at the skin and therefore this number must be minimized. The thermal-to-epithermal-flux-ratio should be 0.05. Nievaart [2] concludes in his thesis that having three neutron beams, one nearly thermal (5 eV) and two epithermal (500 eV and 10 keV), assures an optimal treatment beam, no matter what the influencing biologically weighted dose parameter values may be.

IV. Ration between the total neutron current and the total neutron flux

This ratio provides a measure of the fraction of neutrons that are moving in the forward direction. If only the positive direction is taken into account, the value is between 0-1. A high value is important for two reasons: i) to limit the divergence of the neutron beam and thereby minimize irradiation of surrounding tissue and ii) to permit flexibility in the patient

positioning along the beam central axis. If the current-to-flux-ratio is close to one means that the epithermal flux near the beam exit will change only slightly with distance from the exit. A target number of this ratio should be greater than 0.7.

1.4.3. Dose components

Human tissue consists mainly of hydrogen, oxygen, carbon and nitrogen. Since H and N have the highest microscopic cross section in comparison with O and C, most reactions of neutrons are with H and N. In Appendix A1. Most common isotopes in human body the four cross section plots are given for the most commonly occurring isotopes in the human body. Together with the presence of boron (see Figure 1-1) in human tissue, the majority of the total physical dose considered by BNCT is delivered by H, N and ^{10}B, according to V.A. Nievaart [2].

In Table 1-1 the four major dose components are given. There are four components, since H has two different types of reactions. The second type is a consequence of the fast neutrons which are still present in the incoming neutron beam. This is the reason why the fast neutron component in the neutron beam must be minimized. The thermal neutron flux should also be minimized since, according to Table 1-1, it gives a dose outside the malignant tissue (it reacts with H and N).

Table 1-1 Overview of the four major dose components in BNCT [2].

Physical dose name		Dose symbol	Reaction type	Reaction products	Remarks
Thermal	Boron dose	$\boldsymbol{D_B}$	n,α	$^{10}B + {}^{1}_{0}n \rightarrow {}^{7}Li + {}^{4}He$	Biological effects in tumour and normal tissue are related to ^{10}B micro-distribution
	Thermal neutron dose	$\boldsymbol{D_p}$	n,p	$^{14}N + {}^{1}_{0}n \rightarrow {}^{14}C + {}^{1}_{1}p$	Induced proton 620 keV
	Induced gamma-ray dose	$\boldsymbol{D_\gamma}$ (~2x10^{-13} Gy cm^2 n_{th}^{-1})	n,γ	$^{1}H + {}^{1}_{0}n \rightarrow {}^{2}H + \gamma$	Induced γ-rays 2.2 MeV
Fast	Fast neutron dose	$\boldsymbol{D_n}$ (~2x10^{-13} Gy cm^2 n_{th}^{-1})	n,n	$^{1}H + {}^{1}_{0}n \rightarrow {}^{1}_{0}n + {}^{1}_{1}p + {}^{0}_{-1}e$	Energy recoiling proton is on average half the neutron energy

In Figure 1-3 a schematic is given of the current neutron filter used for BNCT at the High Flux Reactor (HFR) in Petten (NL) together with the fluxes and gamma dose rate in air.

Table 1-2 Beam characteristics and power of five different types of reactors[5].

Reactor	Power (MW)	Φ_{epi} (cm^{-2}s^{-1})	D_n/Φ_{epi} (Gycm^2/n)	D_γ/Φ_{epi} (Gycm^2/n)
HFR	45	3.3e8	8.6e-13	1.0e-12
BMRR	3	1.8e9	4.3e-13	1.3e-13
BMRR (FCB)	3	1.2e10	2.8e-13	1.0e-13
MITR-II	5	2.1e8	8.6e-13	1.3e-12
MITR-II (FCB)	5	1.7e10	1.3e-13	1.0e-13

[5] www.janleenkloosterman.nl

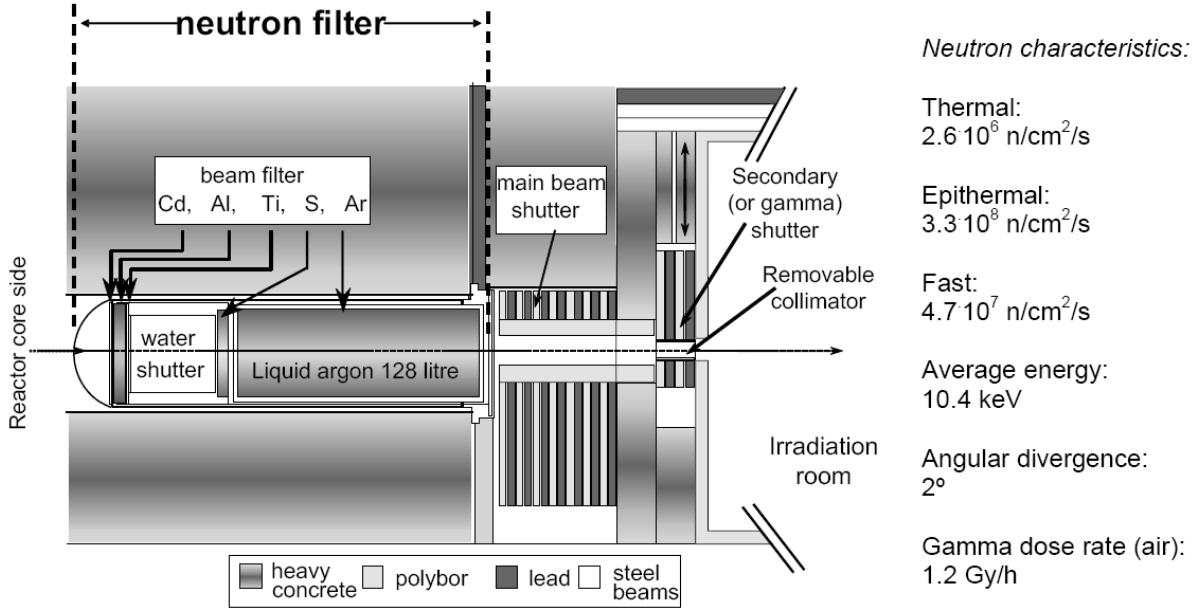

Figure 1-3. A schematic of the current neutron filter for BNCT at the High Flux Reactor in Petten [2].

1.5. Scope of this thesis

According to section 1.3, the spectral tailoring consists of two parts, where in the fist part there have to be found the appropriate neutron energies for irradiation and the second part is how they can be obtained using the right set-up and materials in the filter. In Figure 1-4 a typical spectrum shift arrangement is given [1]. The first part of the spectral tailoring deals with a given neutron spectrum in the tumor and calculate back to point (4) in Figure 1-4. This gives the numbers for thermal, epithermal and fast neutron fluxes given in section 1.4 and is the condition to which the filter must suffice. This was part of Nievaart's thesis.

Part (1) in Figure 1-4 is the filter/ moderator (FM) arrangement[6]. Mostly, the neutron beam measured in (2) is too wide and has a too large divergence, therefore a collimator (3) will narrow the beam and will give it a better *current-to-flux-ratio* (section 1.4.2). Since I will only take the 1-D beam into account, I will leave out the collimator and measure the flux in (2), given a certain filter/ moderator arrangement. This thesis deals with the question to find the optimal materials, number of materials and thicknesses of those materials which could be used in the filter/ moderator arrangement.

[6] During this thesis I will also use filter/ moderator set up or filter/ moderator specification to refer to the filter/ moderator arrangement.

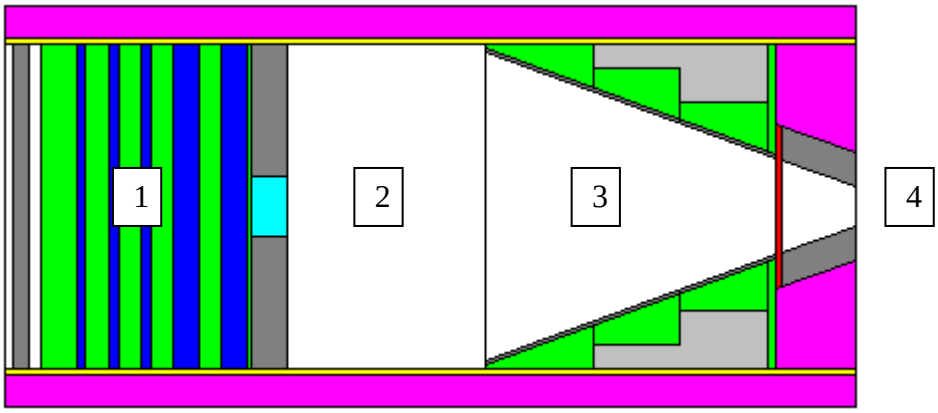

Figure 1-4. Typical spectrum shift arrangement [1].

2. Neutron Filtering

2.1. Introduction

This chapter can roughly be split into two parts. The first part consists of paragraph 2.2 and 2.3. Paragraph 2.2 provides some introductory concepts of nuclear reactor physics while paragraph 2.3 will introduce the neutron transport equation for the one-speed diffusion model. These two paragraphs are mostly a summary of a part of the class *Nuclear Reactor Physics (AP3341 D)* given at TU Delft and the book *Nuclear Reactor Analyses* by *Duderstadt* and *Hamilton* [8]. Secondly, in paragraph 2.4 the characteristics of the filter/ moderator (FM) arrangement will be determined with the concepts of the previous two paragraphs in mind. At last, a list of materials which could be used in the FM arrangement will be given.

2.2. Physics of neutron filtering

This section is partly a brief outline taken from section 2.I.B from Duderstadt and Hamilton [8] and will provide background information about neutron nuclear interactions which occurs in the filter/ moderator arrangement, if while also some introductory theory to choose a selection of materials is given. Here, one can think of the scattering quality or the mean free path of neutrons through materials.

2.2.1. Cross sections

I. Microscopic cross section

When a neutron hits a surface there is a certain probability that it will interact with the nuclei within that surface. That probability is characterized by a quantity called a *nuclear cross section*. If that surface is very thin (say, one atomic layer thick), then no nuclei will be shielded by other nuclei (see Figure 2-1). Now, the interaction rate of the neutrons with the target nuclei is proportional to the intensity of the incoming neutron beam and the number of nuclei. We can write a proportionality constant in front of it and the interaction rate is given by:

$$Rate \equiv R = \sigma I N_A, \tag{2.1}$$

where R is the number of interaction per cm^2 per second. Because the intensity of the incoming neutron beam (I) and the surface density (N_A) is in number per cm^2 per second and number per cm^2 respectively, the proportionality factor has units of area.

If we take a closer look to Figure 2-1 we can say that the cross sectional area[7] should be of order 10^{-24} cm^2. The cross sectional area σ is called the *microscopic cross section* and is in fact measured in *barns* (b), where 1 barn is 10^{-24} cm^2. Note that this interpretation could be misleading, since the fact that the microscopic cross section could be smaller or larger than 1 barn, due to the quantum mechanical nature of the neutron and the nucleus. For example, the absorption cross section of ^{10}B for slow neutrons is almost one thousand times larger than its geometrical cross section.

[7] Since the diameter of a nucleus is in the order of 10^{-12} cm, the geometrical cross sectional area is roughly 10^{-24} cm^2.

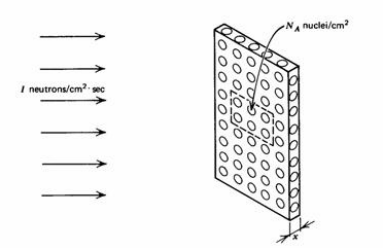

Figure 2-1. A monoenergetic beam incident upon a thin target (Duderstadt and Hamilton)

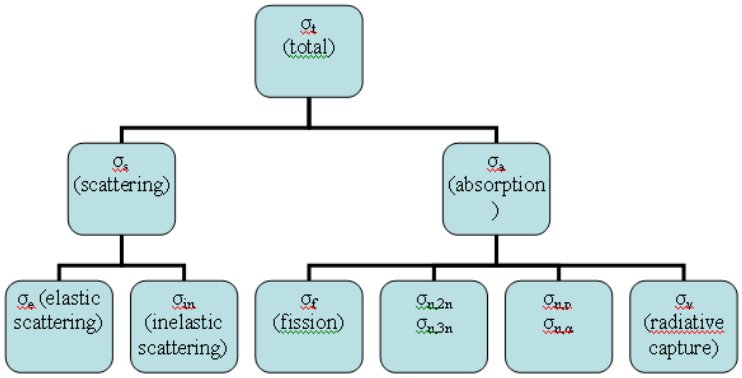

Figure 2-2. Schematic of neutron cross sections.

Since there are several ways in which neutrons can interact with a nucleus, there are also several microscopic cross sections. In Figure 2-2 this hierarchy is shown. Here we can see that scattering consist of elastic and inelastic scattering, where elastic scattering means that the target nucleus remains in its ground state and inelastic scattering means that the target nucleus remains in an excited state. Since cross sections are related to probabilities we can just add the elastic and inelastic cross sections and find the total scattering cross section. This is denoted by:

$$\sigma_s = \sigma_e + \sigma_{in}\,. \tag{2.2}$$

The same holds for the absorption cross section, which is denoted by the sum of the total capture and fission cross sections. The total microscopic cross section is just the sum of all individual cross sections and is given by:

$$\sigma_t = \sigma_s + \sigma_a = \sigma_e + \sigma_{in} + \sigma_f + \sigma_\gamma + \sigma_{n,2n} + \sigma_{n\alpha} + \ldots \tag{2.3}$$

II. Macroscopic cross section

So far, we were only concerned what the chance is that a neutron will interact with a one atomic layer thick target. This was called the microscopic cross section. In this case, the intensity of the beam was the same everywhere, but now, when we take a thicker sample, the intensity of the beam will decrease, due to interactions with nuclei. To take the finite thickness into account, take a look at the following case given schematically in Figure 2-3. At position x the intensity of the beam is $I(x)$ and some infinitesimal distance further the intensity is $I(x+dx)$. And since dx is very small, we know, from earlier observations of thin targets what the interaction rate is within that very small volume. Notice that the number of target nuclei between x and $x+dx$ is given by $dN_A=Ndx$, where N is the number of nuclei per unit volume in the target, we can say that the total reaction rate per unit area in dx is given by:

$$dR = \sigma I dN_A = \sigma I N dx \tag{2.4}$$

.

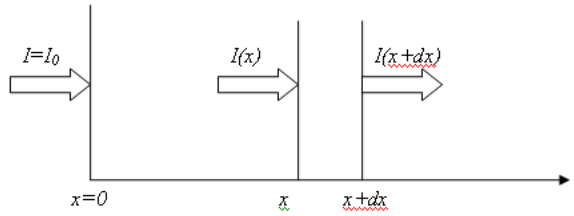

Figure 2-3. A monoenergetic neutron beam incident on a target with finite thickness.

We have not said anything about the cross section used and so, we can just use the total microscopic cross section to calculate the chance in beam intensity between x and $x+dx$. Since the number of interactions is just an indication of the chance in intensity, we can write Eq. (2.4) as:

$$-dI(x) = -\left[I(x+dx) - I(x)\right] = \sigma_t I N dx\,. \tag{2.5}$$

Dividing by dx we find the differential equation for the beam intensity $I(x)$:

$$\frac{dI(x)}{dx} = -N\sigma_t I(x)\,. \tag{2.6}$$

If we solve this equation by applying that at the boundary $x=0$ the intensity of the beam is I_0, we find an exponential decay of the beam intensity with respect to x:

$$I(x) = I_0 \exp\left(-N\sigma_t x\right). \tag{2.7}$$

The product of the atomic density with the microscopic cross section is so frequently used that they give it a special symbol:

$$\Sigma_t = N\sigma_t = \left[\frac{\#}{cm^3}\right]\left[cm^2\right] = \left[\frac{1}{cm}\right]. \tag{2.8}$$

This is called the *macroscopic cross section* and is a property of the target material.

III. Characteristics of neutron-nuclear cross sections

In the previous two sections we have discussed the probabilities that a neutron will interact with target nuclei. It should be obvious that certain probabilities are dependent on what nuclei are used as the target. It will go too far to discuss this in much detail, but there are some remarks I would like to make.

a) Mean Free Path

Since the intensity of the neutron beam in a certain material, characterized by the total cross section Σ_t, decreases by the relation given in Eq. (2.7), the chance of no interaction is:

$$P(x) = \exp\left(-\Sigma_t x\right). \tag{2.9}$$

With this relation in mind, we can simply calculate the mean free path before interaction by weighing each length by the chance of no interaction:

$$\lambda = \frac{\int_0^\infty xP(x)\,dx}{\int_0^\infty P(x)\,dx} = \frac{\int_0^\infty x\exp(-\Sigma_t x)\,dx}{\int_0^\infty \exp(-\Sigma_t x)\,dx} = \frac{1}{\Sigma_t}. \tag{2.10}$$

So the mfp is just the inverse of the total cross sectional area.

b) Scattering Quality

We would like to slow neutrons down with nuclei with a certain mass number *A*. With the conservation of momentum and energy we can simply obtain a relation for which mass numbers are good to use as a moderator. Momentum conservation and energy conservation are respectively:

$$\begin{aligned} v_{n,before} &= v_{n,after} + Av_m \\ \frac{1}{2}\left(v_{n,before}\right)^2 &= \frac{1}{2}\left(v_{n,after}\right)^2 + \frac{1}{2}A\left(v_m\right)^2, \end{aligned} \tag{2.11}$$

Where the index *m* stands for the moderator with mass number *A*. Note that we have neglected the mass difference between the protons and the neutrons within the nuclei of the moderator, so that we can approach the mass of the moderator nuclei of *A* times the mass of a neutron[8].

If we now calculate the energy for the neutron after a collision with a moderator nucleus, we see that:

$$\frac{\frac{1}{2}\left(v_{n,before}\right)^2 - \frac{1}{2}\left(v_{n,after}\right)^2}{\frac{1}{2}\left(v_{n,before}\right)^2} = \frac{4A}{(1+A)^2}. \tag{2.12}$$

Since this relation has its highest values for low numbers for *A*, it's best to use light nuclei as moderator, because the neutrons will loss most of their energy.

In literature you'll sometimes find the following relation for the moderating quality or ratio:

$$\text{Moderating ratio} \equiv \frac{\xi\Sigma_s}{\Sigma_a}, \tag{2.13}$$

[8] The mass of a neutron (m_n) is $1.6749*10^{-27}$ kg of a proton (m_p) is $1.6726*10^{-27}$ kg. If we neglect the mass difference between m_n and m_p, which is approximately $0.02*10^{-27}$ kg, we obtain for Bismuth (atomic number 83) a mass which is 83 times $0.002*10^{-27}$ kg heavier than we would find in literature. This is approximately 1/8 times the mass of one neutron and less then one per cent of the total mass of Bismuth.

Where ξ corresponds to the average logarithmic energy loss of a neutron in a collision with a nucleus of arbitrary mass number:

$$\xi = 1 + \frac{\alpha}{1-\alpha}\ln\alpha = 1 - \frac{(A-1)^2}{2A}\ln\left(\frac{A+1}{A-1}\right). \tag{2.14}$$

Here $\alpha = \left(\frac{A-1}{A+1}\right)^2$. Though, a good approximation for de moderating quality is just:

$$\text{Moderating quality} = \frac{\Sigma_s}{\Sigma_a}, \tag{2.15}$$

where a large number indicates a good moderator.

c) Absorption

It's already mentioned that big resonances in the cross sections are due to quantum mechanical effects. Those resonances are narrow peaks which are separated by very narrow gaps. Those peaks are a consequence of so-called *resonance reactions* [8], which means that an incident neutron has energies equal to that of one of the energy levels of the target nucleus. Since larger nuclei have more energy levels, they are better absorbers. For a more detailed observation of cross sections and its characteristics I refer to section 2. I. C.1-2 of Duderstadt & Hamilton [8].

d) Interaction

In Figure 2-2 the various types of neutron-nucleus interactions are given. The simplest way of interaction is what is called *potential scattering*, where the neutron hits a nucleus like a billiard ball hits another billiard ball (it just bounces of the nucleus without penetrating the nuclear surface). Such billiard-ball collisions are characterized by essentially energy-independent cross sections in the order of magnitude of the geometric cross section of the nucleus.

For the other types of interaction the neutron does penetrates the surface. During the time the neutron is absorbed by the nucleus, an intermediate nucleus is formed[9]. Such an intermediate nucleus can decay in various ways, such as given by:

$${}^{1}_{0}n + {}^{A}_{Z}X \rightarrow \left({}^{A+1}_{Z}Z\right)^{*} \begin{cases} {}^{1}_{0}n + {}^{A}_{Z}X & \text{Resonance elastic scattering} \\ {}^{1}_{0}n + \left({}^{A}_{Z}X\right)^{*} & \text{Inelastic scattering} \\ {}^{A+1}_{Z}Z + \gamma & \text{Radiative capture} \\ {}^{A1}_{Z1}X + {}^{A2}_{Z2}X + 2 - 3\,{}^{1}_{0}n & \text{Fission} \end{cases} \tag{2.16}$$

[9] Since a slow neutron travelling at 10^5 cm/s would take some 10^{-17} sec. to pass a neutron and a neutron-nucleus interaction such as fission takes some 10^{-14} sec. there must be some intermediate nucleus to delay the whole process.

2.3. Neutron transport

2.3.1. Transport equation

I. Neutron transport equation - general

It goes beyond the scope of this thesis to derive the neutron transport equation. For readers whom are interested, I refer to Duderstadt & Hamilton for a clear derivation [8]. From now on, I will just give the neutron transport equation:

$$\frac{\partial n}{\partial t} + v\underline{\Omega}\cdot\underline{\nabla}n + v\Sigma_t n\left(\underline{r},E,\underline{\Omega},t\right) = \int_{4\pi} d\underline{\Omega}' \int_0^\infty dE' v'\Sigma_s\left(E'\to E,\underline{\Omega}'\to\underline{\Omega}\right) n\left(\underline{r},E,\underline{\Omega},t\right) \quad (2.17)$$

II. Neutron transport equation - 1D case

In this thesis the interest goes out to the one-dimensional case, so suppose the neutrons are only traveling in the *x*-direction. Eq. (2.17) becomes a little bit less abstract, since the derivative in the *x*-, *y*- and *z*-direction becomes only a derivative in the *x*-direction, and Ω_x becomes $cos\Theta$, where $cos\Theta=1$ means that the neutron beam is parallel to the *x*-direction and $cos\Theta=0$ means that the neutrons travel perpendicular to it.

The one-dimensional neutron transport equation becomes:

$$\begin{aligned}&\frac{1}{v}\frac{\partial\varphi}{\partial t} + \cos\theta\frac{\partial\varphi}{\partial x} + \Sigma_t\varphi\left(x,E,\theta,t\right)\\ &\qquad = \int_0^\pi d\theta' \sin\theta' \int_0^\infty dE'\Sigma_s\left(E'\to E,\theta'\to\theta\right)\varphi\left(x,E',\theta',t\right)\end{aligned} \quad . \quad (2.18)$$

Note that this equation is written in terms of the angular flux. Where the angular flux is given by:

$$\varphi\left(\underline{r},E,\underline{\Omega},t\right) \equiv vn\left(\underline{r},E,\underline{\Omega},t\right). \quad (2.19)$$

Now, the time derivative of the neutron population can simply be obtained by differentiating Eq. (2.19).

To rewrite Eq. (2.18) to its final form it's useful to define a new variable $\mu=cos\Theta$. Note that as Θ ranges between 0 and π, μ ranges between -1 and 1. Hence the usual form of the one-dimensional transport equation can be written as:

$$\begin{aligned}&\frac{1}{v}\frac{\partial\varphi}{\partial t} + \mu\frac{\partial\varphi}{\partial x} + \Sigma_t\varphi\left(x,E,\mu,t\right)\\ &\qquad = \int_{-1}^{+1} d\mu' \int_0^\infty dE'\Sigma_s\left(E'\to E,\mu'\to\mu\right)\varphi\left(x,E',\mu',t\right) + s\left(x,E,\mu,t\right)\end{aligned} \quad (2.20)$$

2.4. Characteristics

The neutron energy spectrum can roughly be cut in three energy regions: thermal, epithermal and fast. In section 1.2.1 the energy boundaries of these regions are defined. According to

V.A. Nievaart [2], most neutrons should be in the epithermal region[10] and according to the IAEA-tecdoc [1] discussed in section 1.4, the gamma contamination should be minimized. Therefore several materials could be used to obtain for an arbitrary incoming neutron beam an out coming neutron beam with a maximum around the epithermal neutron energies and with a low number of gamma radiation. This section provides a list of materials which could be used in the filter/ moderator arrangement.

2.4.1. Filter/ Moderator characteristics

According to section 1.2.1 the irradiation beam intensity should have its maximum around epithermal neutron energies. According to Eq. (2.15), the moderating quality decreases when absorption cross section of materials in the filter increases. Therefore, materials with low absorption cross sections for all neutron energies except in the thermal energy range[11] must be used. In Table 2-1 these characteristics per energy region are given.

Table 2-1 Cross section characteristics of the materials for the filter/ moderator arrangement separated in three different energy regions[12]

	Energy range	Characteristics
Thermal	0 – 5 eV	• High absorption cross section • High scatter cross section
Epithermal	5 eV – 10 keV	• Low scatter cross section • Low absorption cross section
Fast	10 keV – 20 MeV	• High scatter cross section • Low absorption cross section

Other criteria the materials in the filter/ moderator arrangement should meet are[13]:

a. The materials should not undergo phase changes,
b. The material should not decompose or emit toxic substances in the radiation beam,
c. The material should not accumulate high long-term radioactivity and activation,
d. The material should not contain impurities or moisture,
e. The materials should not be too expensive,
f. The arrangement should be ‘easy’ to build and maintain.

2.4.2. Materials

The filter should reduce the gamma ray contamination, thermal neutron current and the fast neutron current contamination. Therefore the filter can be split into three parts given in Figure

[10] Nievaart did conclude that besides the 10 keV epithermal neutrons, low epithermal neutrons of around 1 eV and thermal neutrons with energies of 0.1 eV must also be used.
[11] Since neutrons with thermal energies can not be up scattered to higher energies these neutrons must be filtered out the neutron beam.
[12] Note that this is not the true definition of *thermal*, *epithermal* and *fast*. This definition of the three different energy regions was used to obtain a simple goal function which is the *thermal* neutron current divided by the total neutron current.
[13] http://www.janleenkloosterman.nl/.

2-4, where each part consists of different materials with different characteristics in moderating and or absorbing neutrons or gamma radiation.

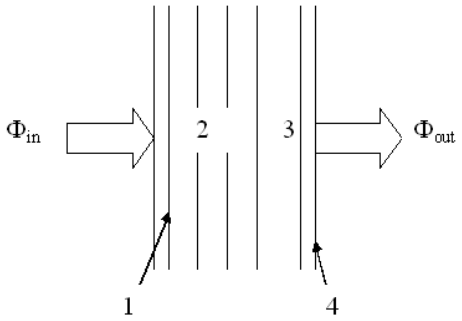

Figure 2-4 **A schematic of the filter/ moderator arrangement. The filter is split into three parts, where part 1 and 4 reduces the gamma contamination, part 2 reduces the fast neutron current contamination and part 3 reduces the thermal neutron current contamination.**

Part 1 and 4 contain materials to reduce the gamma radiation, where part 1 filters the gamma contamination coming from the neutron source and part 4 filters the gamma rays produced in the filter by radiative capture (Figure 2-2) . Part 1 is optional[14]. Part 2 consists of materials to reduce the fast neutron current contamination where part 3 consists of materials that reduce the thermal neutron current contamination. Every part has its own specific materials and should be placed in that typical order (i.e. first moderate the fast neutron current before filtering the thermal neutrons), because when part 2 moderates the fast neutron content, thermal neutrons are 'formed' and therefore thermal neutrons must be filtered after the fast neutron moderation. In appendix A cross section plots are given. In Table 2-2 the characteristics and the costs of materials which could be used in the FM arrangement are given.

In the following three subsections a clarification of the materials shown in Table 2-2 will be given.

I. Gamma ray contamination

Gamma rays can give a high toxic dose to the human body. Two materials which are good gamma absorbers are lead and bismuth. Bismuth has a higher transmission (i.e. lower absorption) for epithermal neutrons, but caution is needed in handling neutron-irradiated bismuth, because of the buildup of ^{210}Po. Encapsulation of the bismuth is highly recommended. The buildup of ^{210}Po also changes the total cross section of the filter/ moderator arrangement, and therefore the quality of the filter/ moderator is not constant in time. When bismuth is used in the filter, criteria c. and d. are not satisfied and also the costs of bismuth compared to lead is approximately ten times higher (see Table 2-2).

To protect the people within the irradiation room for gamma rays steel and iron could be used. To protect the steel and iron for the gamma rays, shielding containing ^{10}B or ^{6}Li could be used.

II. FAST NEUTRON CURRENT CONTAMINATION

According to Table 1-1 fast neutrons will give a toxic dose to the human body and since most neutrons from the neutron source have energies in the fast energy range, the fast neutrons

[14] Since the gamma rays from the neutron source could influence the materials in the filter/ moderator arrangement its better to reduce those gammas, but it should be investigated whether the advantage of less incoming gammas does not influence the quality of the FM arrangement.

must be slowed down by materials with high scatter cross sections in at least the high energy range. Fast neutrons should not being captured since the intensity of the irradiation beam will be very low, therefore fast neutrons must be moderated to remain a high intensity.

According to section 2.2.1 (Eq. 2.12) good moderators, or scatterers, are materials with mass numbers compared to the mass number of a neutron. For example, B-10 is a material that fulfills this criteria, but isn't in fact a good moderator, since it has a very high absorption cross section in the thermal range and a low absorption cross section in the fast range. According to Eq. (2.15) the moderating quality is the ration between scatter and the absorption cross section, in appendix A3 this moderating quality for several natural elements is given. A moderating quality in the range of 10^4-10^5 is good, where B-10 has a moderating quality less then one means that it hasn't good capabilities of slowing down the neutrons.

Combinations of Al followed by Al_2O_3 or AlF_3 downstream, i.e. near the beam exit, are very efficient moderators, because the O and F cross-sections fill in the valleys between the energy resonance peaks of Al (see Figure 2-5). In Figure 2-5 to Figure 2-7 the scatter and capture cross sections and the moderating quality are given for aluminum, oxygen and fluoride respectively, where in Figure 2-8 the moderating quality of Al_2O_3, AlF_3 and H_2O given. From Figure 2-8 it can be seen that AlF_3 is a better moderator for neutron energies less then 10 keV, where Al_2O_3 is a better moderator for fast neutron energies (higher then 10 keV). Just for comparison the cross section of water is added to the graph.

In Appendix A3 the moderating quality of other possible moderators is given.

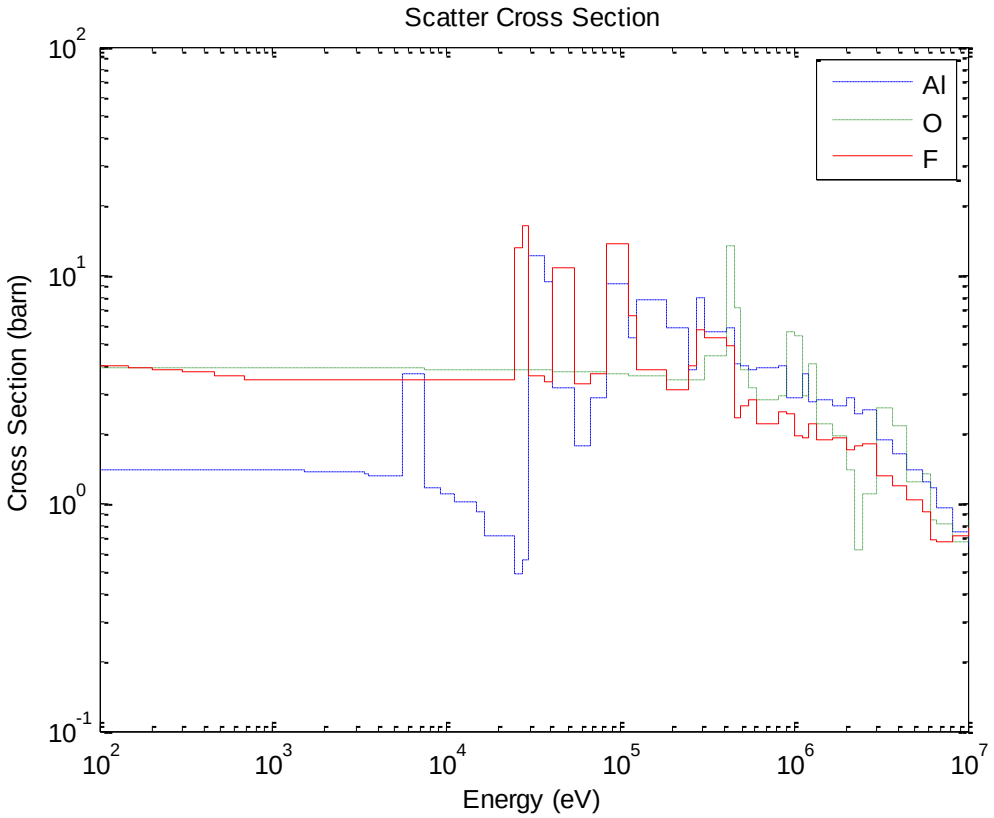

Figure 2-5 **The scatter cross section of aluminum, oxygen and fluoride. Here it can be seen that oxygen and fluoride cross sections fill in the valleys between the energy resonance peaks of aluminum.**

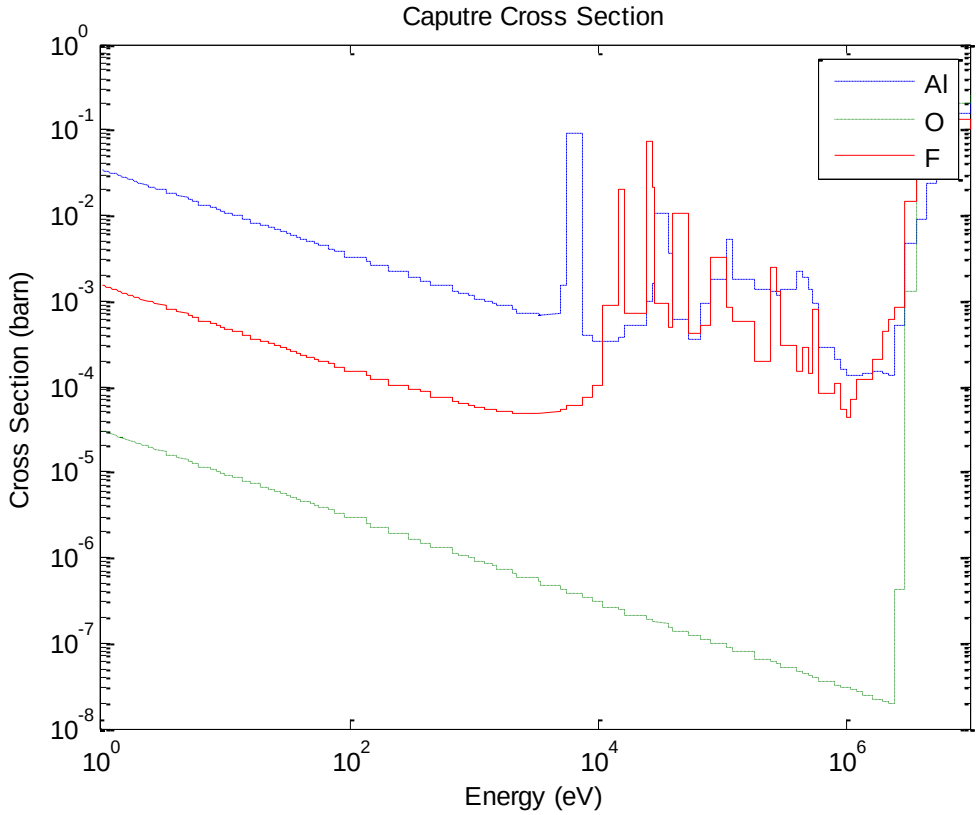

Figure 2-6 **The capture cross section of aluminum, oxygen and fluoride. Here it can be seen that oxygen and fluoride cross sections fill in the valleys between the energy resonance peaks of aluminum, though the capture cross section of oxygen is much smaller than of aluminum.**

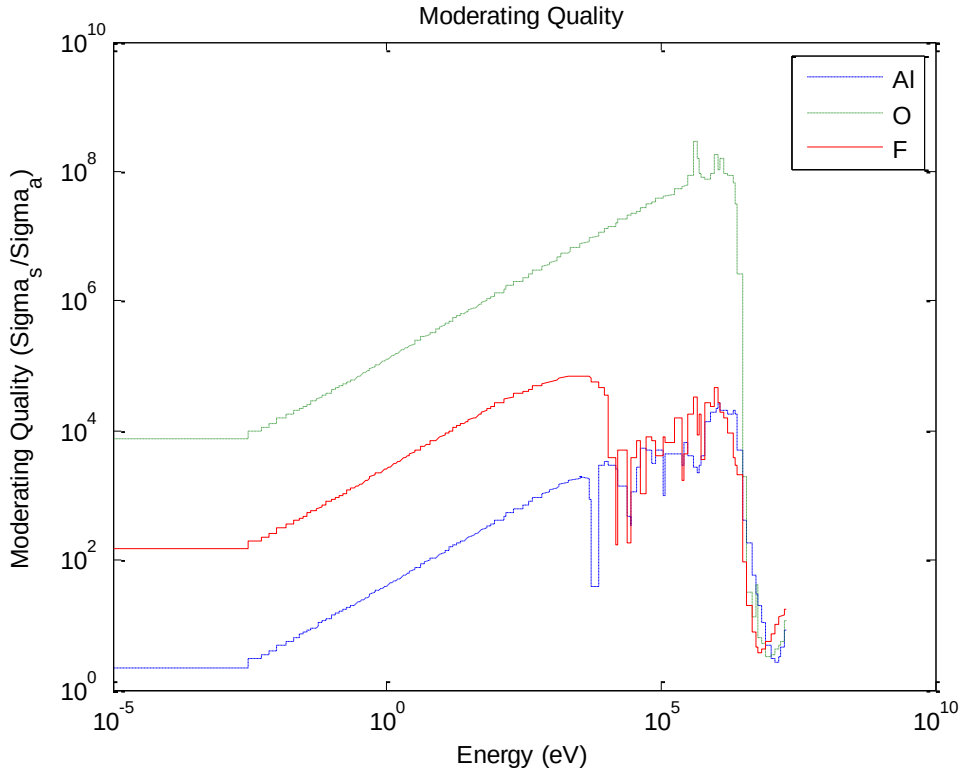

Figure 2-7 **The moderating quality of aluminum, oxygen and fluoride. Since oxygen has a much smaller capture cross section, the moderating quality of oxygen is better than of aluminum and fluoride.**

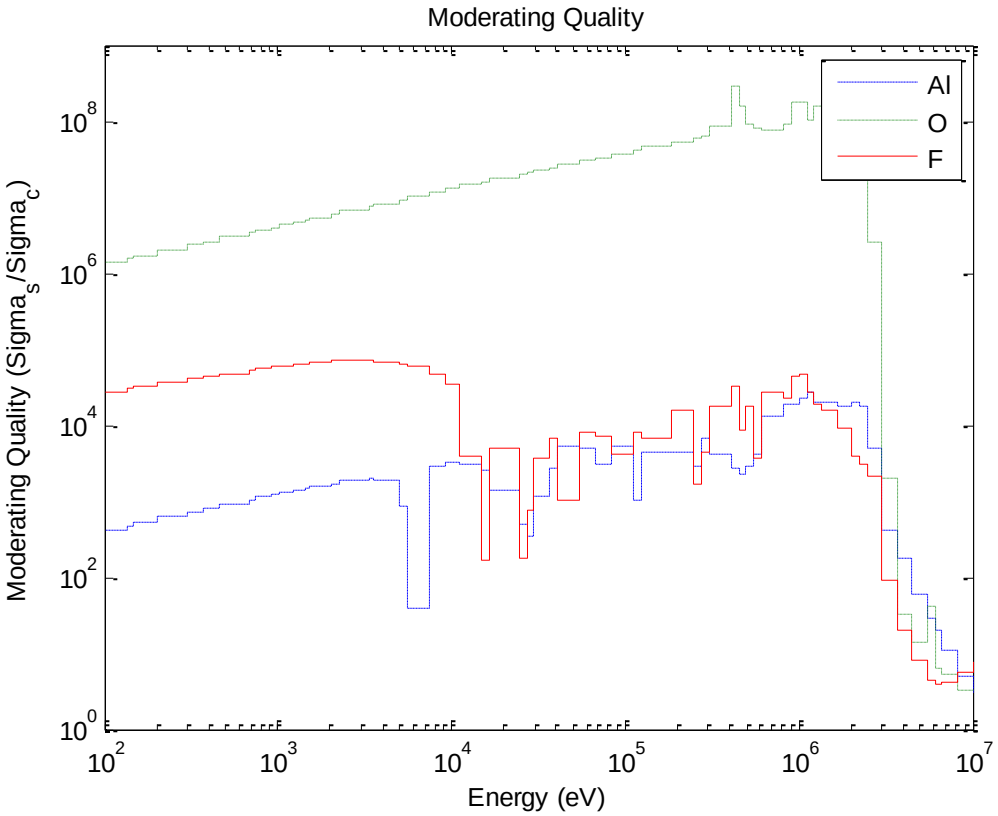

Figure 2-8 The moderating quality of Al_2O_3, AlF_3 and H_2O.

III. Thermal neutron current contamination

When the boron carrier is added to the patient, there also will be some boron outside the tumor in the healthy tissue. Due to this fact thermal neutrons in the irradiation beam will give a high (toxic) dose in the healthy tissue and therefore the thermal neutron population in the incident beam must be minimized, or at least, according to Nievaart [2] be very small.

Elements which are good thermal neutron absorbers are: He-3, B-10, Li-6, N-14 and Cl. But since He-3 is very rare, an abundance of 0.000138% in the earth's crust, and it has a high potential as an energy source, it's not very useful as a thermal neutron absorber.

Lithium is nearly ten times cheaper as boron, but also almost five times less in absorbing thermal neutrons. Nitrogen and chlorine could also be used, but since they are gasses they must be held at very low temperatures to obtain a high density and a high macroscopic cross section (note that the macroscopic cross section is the microscopic cross section times the density, Eq. (2.8))

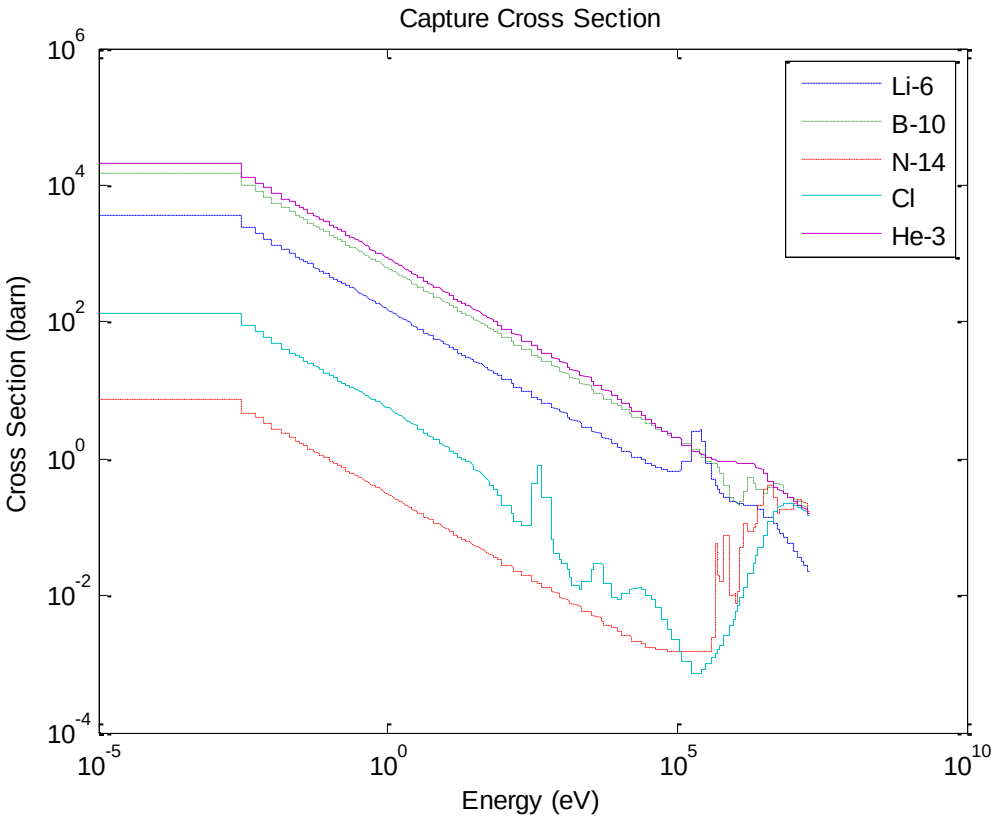

Figure 2-9 **Some capture cross sections of potentially thermal neutron absorbers.**

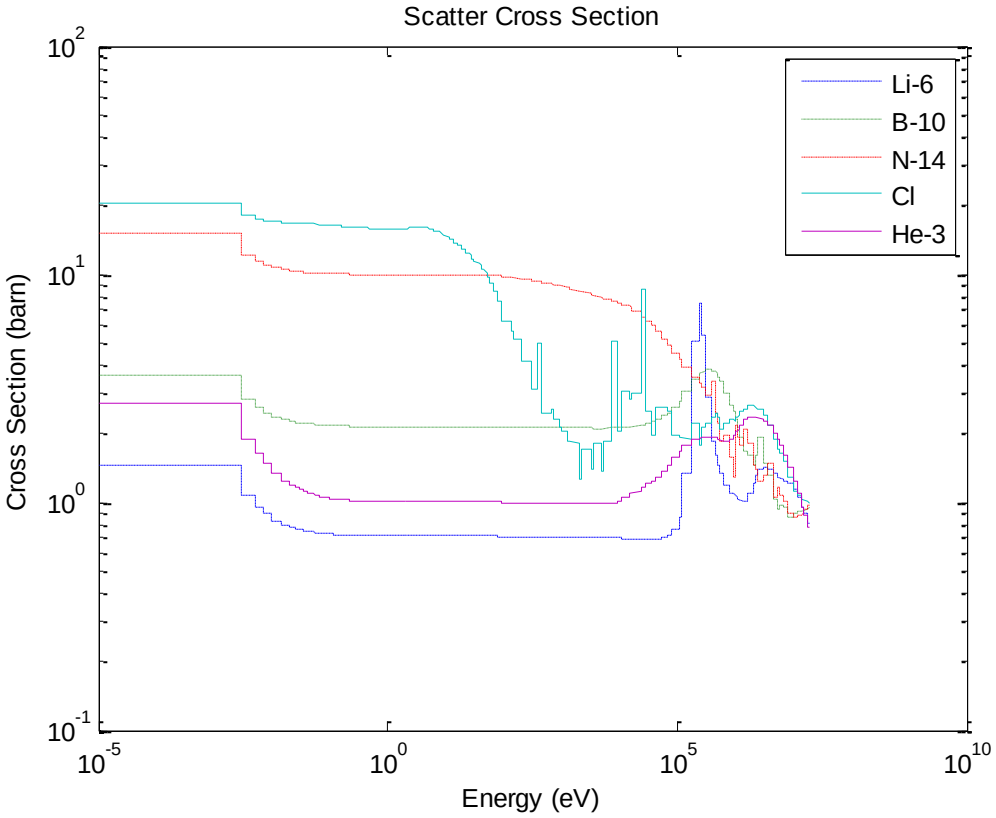

Figure 2-10 **Some scatter cross sections of potentially thermal neutron absorbers.**

Table 2-2 Elements with their properties and costs (http://www.chemicool.com/elements/lithium.html, May 2008). The elements indicated in bold are good for use as thermal neutron absorbers, where the elements indicated in *italic* are good for use as gamma ray absorbers. The elements indicated in normal letter type are good for use as fast neutron moderators.

Elements (#, Z)	State at 293 K	Melting point (K)	Boiling point (K)	Density at 293 K (g/cm^3)	Toxicity	Costs, pure ($/100 g)
Aluminum (Al, 13)	s	933.57	2740	2.7	-	1.8
Argon (Ar, 18)	g	84	87.3	0.00178	no	0.5
Beryllium (Be, 4)	s	1551.2	2773	1.848	yes	530
Bismuth (Bi, 83)	*s*	*544.5*	*1837*	*9.8*	-	*11*
Boron (B, 5)	**s**	**2352.2**	**3923.2**	**2.34**	**-**	**250**
Carbon (C, 6)	s	3823.2	-	2.62	-	2,4
Chromium (Cr, 24)	s	2130.2	2963	7.19	-	10
Chlorine (Cl, 17)	**g**	**172,22**	**239.2**	**0.00321**	**yes**	**0.15**
Fluorine (F, 9)	g	53.58	85.1	0.00170	yes	190
Gold (Au, 79)	s	1337.63	3081	19.32	-	4400
Helium (He, 2)	**g**	**-**	**4.2**	**0.00018**	**no**	**5.2**
Hydrogen (H, 1)	g	14.06	20.4	0.00009	-	12
Iron (Fe, 26)	s	1808.2	3023	7.86	-	6,7
Lead (Pb, 82)	*s*	*600.7*	*2024*	*11.34*	-	*1.5*
Lithium (Li, 3)	**s**	**453.7**	**1620**	**0.53**	**-**	**27**
Magnesium (Mg, 12)	s	922	1378	1.738	-	3.7
Manganese (Mn, 25)	s	1517.2	2333	7.43	-	1.7
Nickel (Ni, 28)	s	1726.2	3193	8.90	yes	7.7
Nitrogen (N, 7)	**g**	**63.34**	**77.4**	**0.00125**	**no**	**0.4**
Oxygen (O, 8)	g	54.8	90.2	0.00143	no	0.3
Phosphorus (P, 15)	s	317.3	553.7	1.82	yes	4
Silicon (Si, 14)	s	1683.2	3553	2.33	-	5.4
Sulfur (S, 16)	s	386	717.9	2.07	-	24
Tin (Sn, 50)	s	505.168	2896	7.30	-	8
Titanium (Ti, 22)	s	1933.2	3558	4.50	-	6.1
Xenon (Xe, 54)	g	161.3	165	0.00588	no	120
Zirconium (Zr, 40)	s	2125.2	4473	6.4	-	16

3. Calculation Methods

3.1. Introduction

This chapter will provide the method used for the optimization. For neutron transport through materials the Monte Carlo N-Particle (MCNP5) Transport code has been used [10, 11, 12]. In paragraph 3.2 an explanation of an MNCP input file will be given. Also the method for measuring the neutrons and how to interpret the output data of MCNP will be given in this paragraph. In paragraph 3.3 the optimization method will be discussed. In this part, the goal function will also be introduced. The optimization code is written in Perl and the scheme of the Perl script will also be discussed in this paragraph. Finally, in the last section, paragraph 3.4, the measuring method will be discussed. In this section I will give some filter/ moderator specifications which will be investigated by use of the optimization script.

3.2. Monte Carlo calculation

This section will provide an explanation of the MCNP input file used for this thesis.

3.2.1. Introduction

MCNP is developed and owned by the Los Alamos National Laboratory and has a significant history dating to the early years of the Manhattan Project, there it was primarily used for the simulation of nuclear processes, such as fission. Nowadays, MCNP has been used successfully to solve many problems in the field of medical physics, since it has the capability to simulate particle interactions involving neutrons, photons and electrons [10, 13].

3.2.2. MCNP script

The MCNP code is used for modeling neutron transport in the filter. An MNCP input file has always the following form [11]:

Message Block (optional)
Blank Line Delimiter (optional)
One-line Problem Title Card
Cell Cards
••
Blank Line Delimiter
Surface Cards
••
Blank Line Delimiter
Data Cards
••
Blank Line Terminator (optional)

In Appendix B. MCNP Code the MCNP input code used for this thesis is given. In the next three subsections some comments will be given to each part in the MCNP input file, i.e. the cell, surface and data cards.

I. Cell cards

With cell cards the cells of a structure used in a problem are defined. A cell could be a sphere, or in this thesis, blocks successively put together. In the MCNP code these blocks are defined by the following five lines (which means that there are five cells and four blocks in this problem, since one cell contains the outer space, i.e the space which is not enclosed by the blocks):

```
1  0          1 -2 6 -7 8 -9 imp:n=1
2  1  -2.91   2 -3 6 -7 8 -9 imp:n=1
3  2  -2.340  3 -4 6 -7 8 -9 imp:n=1
4  0          4 -5 6 -7 8 -9 imp:n=1
5  0          -1:4:-5:6:-7:8 imp:n=0
```

Each line defines the cell in the following order. First a number is added to the cell, this is called the cell number. The second number indicates whether the cell is a void (given by a 0) or contains a material (given by any number with a maximum of five digits), if the cell is a void we can directly say by which surfaces the cell is bounded, if the cell contains a material the density of that material must be given in either g/cm^3 or 10^{24} atoms/cm^3. If the density is given like *-2.91* means that it has units g/cm^3, if the density is given like *2.91* means that is has units 10^{24} atoms/cm^3. For example, cell 2 contains a material (the second number is not a zero) with a density of 2.91 g/cm^3 and the material is called material 1, that refers to a *material card* further on in the MCNP script. Cell 2 is bounded by surfaces 2, 3, 6, 7, 8 and 9, how those surfaces are defined follows in the next subsection.

In Figure 3-1 the top view of the filter/ moderator set up is given, in here each cell number is enclosed by a circle and each surface number is placed above each line. Surface 6 and 7 are the top and bottom of this cube and lie in the xz plane. In two dimensions (in the xz plane), cell 1 is enclosed by 'boundary' lines 1, 2, 8 and 9 and is the overlapping surface of everything on the right of line 1, the left of line 2, above line 9 and below line 8. In MCNP this is written as: 1 -2 8 -9, where the minus sign means that it's everything from that line in the negative direction perpendicular to that line. In three dimensions each boundary line becomes a boundary surface[15].

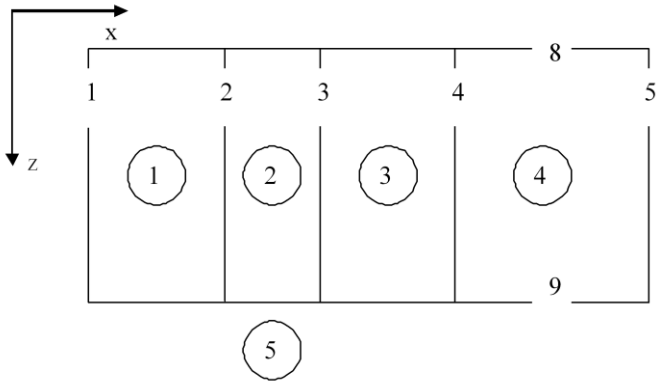

Figure 3-1 **Top view of the filter/ moderator set up. The numbers inside a circle indicate the cell numbers surrounded by the surface indicated by the numbers on top of the lines. Cell number 5 indicates the outside world, i.e. everything except the space inside a cell. The positive y-direction is pointing out the paper.**

[15] A two dimensional cell is bounded by one dimensional lines, where a three dimensional cell is bounded by two dimensional surfaces.

Finally, each line ends with *imp:n=1*[16], which tells MCNP what particles must be tracked in each cell (particle importance), where *n=1* means that the neutron importance is one. In cell 5, the neutron importance is zero, which means that if neutrons enters cell 5, they will be lost.

II. Surface cards

Now when the cells are defined by the boundaries, the boundaries must be further defined. This is done by the surface cards. Note footnote 15 that only three dimensional shapes are bounded by two dimensional surfaces. From Figure 3-1 and Figure 3-3 it can be seen that there are nine boundary surfaces and therefore nine surface cards are needed. These cards are given by:

```
1   PX -5
2   PX 0
3   PX 20
4   PX 21
5   PX 100
6*  PY 0
7*  PY 100
8*  PZ 0
9*  PZ 100
```

Where the first number on each lines defines the surface number and an asterisk means that the surface is a reflecting surface, so no particles can penetrate the surface. If no asterisk is added to the surface number, each particle can penetrate the surface. For example, surface 1 is a penetrating surface, where *PX=-5* means that it's a (infinite) flat surface at *x=-5*. Surfaces 6 to 9 are reflecting surfaces, which mean that the filter/ moderator structure in this thesis is surrounded by reflecting boundaries and neutrons can only reach cell 5 by penetrating through surfaces one and five.

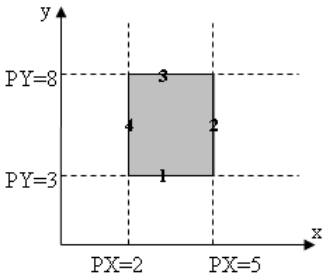

Figure 3-2 A simple example to define a 2-D surface in MCNP.

In Figure 3-2 an example of how to define a surface in MCNP is given in two dimensions. The grey surface is bounded by lines 1, 2, 3 and 4. In MCNP this is defined as follows:

[16] MCNP has different modes. Mode *N*, *P* or *E* means respectively neutron, photon or electron transport only (for this thesis, mode *N* has been used), *N P* stands for neutron and neutron-induced photon transport, *P E* photon and electron transport and finally *N P E* indicates neutron, neutron-induced photon, and electron transport altogether.

Grey surface (*one line problem title card*)
1 0 1 -3 4 -2
(*blank line delimiter*)
1 PY=3
2 PX=5
3 PY=8
4 PX=2

When the cells and surfaces are defined the filter/ moderator set up gets the shape illustrated by Figure 3-3. To give it an easy view, the cell and surface numbers are left out this picture.

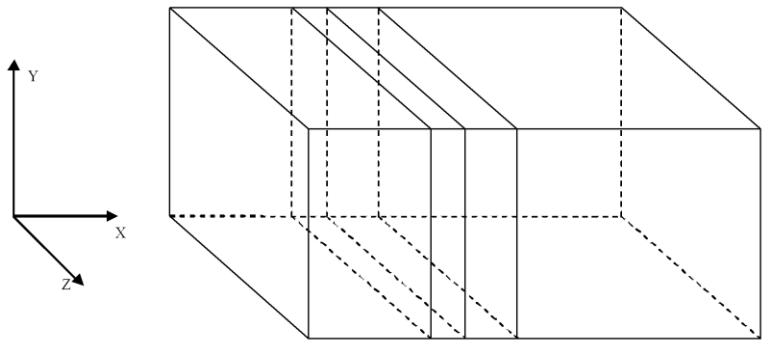

Figure 3-3 **A schematic in 3-D of the filter/ moderator set up. To keep it an easy-view, I have left out the cell and surface numbers. Surface numbers 6 and 7 are at the top and bottom of this figure.**

III. Data cards

The data card is separated in a source definition, tally definitions, energy bins in which there will be tallied, material definitions which are stated in the cell cards and finally a cutoff definition. In MCNP this looks like:

```
SDEF ERG=2 PAR=1 NRM=1 DIR=1 X=-5 Y=D1 Z=D2 VEC=1
SI1  0. 100.
SI2  0. 100.
SP1  0. 1.
SP2  0. 1.
F1:N 5
E1 0.0001 8I 0.001 38I 0.040 5I 0.1 18I 2
F11:N 5
E11 0.000005 0.020 2
M1 13027 0.25 9019 0.75
M2 5010 1
NPS 1000000
PRDMP 1000000 1000000 -1 5 0
```

The source definition line starts with the indication of *SDEF*. The energy of the source is defined by *ERG* in MeV. The type of source is given by *PAR*, where *PAR=1* means that it's a neutron source. The directionality of the beam is indicated by *NRM* and *DIR*, which defines the surface normal and the angle of the beam with respect to that normal respectively. *DIR=1* means that the angle of the cosine equals one. Finally the source must be a plane source at x = -5 which is 100 cm high and width in the y- and z-direction. In the MCNP manual vol. II [11] other source definition are given and specified.

The tally cards are indicated by *Fn*, where n could be 1, 2, 4, 5a, 6, 7 or 8, where each number refers to a different type of detector. In this thesis we are interested in neutron current, which means that tally type *F1* should be used. To tally in different energy regions, energy bins could be introduced by using the energy card, indicated by *En*, where *n* refers to the tally type used. Energy card *E1* relates to tally *F1* and *E2* relates to *F2*. Tally *F1* is the same as tally *F11* or *F14*, this could be useful to measure twice the same, but with different energy bins. The energy bins defined by *E11* relates to tally *F11*.

Material cards are indicated with *Mn*, where the number n relates to the cell where material 1 is defined. For example, in this thesis material 1 is placed in cell 2 and material 2 is placed in cell 3. After the mnemonic *Mn* the material and its fraction in the cell is defined[17]. This is done by: $ZZZAAA_1$ $fraction_1$ $ZZZAAA_2$ $fraction_2$ etc. , where ZZZ is the atomic number and AAA is atomic mass.

Finally we want the problem to terminate after a certain amount of runs and that is done by problem cutoff cards. The *NPS* card is the simplest one and will terminate MCNP after *NPS* histories have been tracked. The *PRDMP* card controls the interval at which tallies are printed to the output file and information is dumped to the *RUNTPE* file. For more detailed information I refer to the MCNP manual.

3.2.3. Tally data

I. Tally type

Mentioned earlier, MCNP has different types of estimators for tallying. For this thesis the current tally (type *F1*) is used and is in MCNP, before the final normalization per starting particle, represented by:

$$J(\mathbf{r}) = \int_{E_1}^{E_2} \int_{4\pi} |\mathbf{n}\bullet\Omega| \phi(\mathbf{r}, E, \Omega) dE d\Omega , \tag{3.1}$$

where E_1 and E_2 are the boundaries of the energy bin.

Tally *F1* measures the current in every bin, so in fact it's sort of a 'group flux', given by:

$$\phi_g = \int \phi(E)\, dE . \tag{3.2}$$

Therefore to give a good measure of the whole energy spectrum, the derivative of the measured current in each bin must be taken, which is equal to the measured current divided by the width of the energy bin:

$$\phi(E) = \frac{d\phi}{dE} = \frac{\phi_g}{\Delta E} . \tag{3.3}$$

This could be done by Matlab or other programs.

[17] Note that a cell can contain more than one material.

II. Error

The measure of the tally is printed in the output accompanied by a second number *R*, which is the relative error. This estimated relative error can be used to form confidence intervals about the estimated mean and according to the law of large numbers the estimated mean converges towards the expected value for *N* goes to infinity. Here *N* is the number of histories done. When *N* approaches infinity there is a 68% chance that the true results will be in the range $\bar{x}(1 \pm R)$ and a 95% $\bar{x}(1 \pm 2R)$. Guidelines for interpreting the quality of the confidence interval for various values or *R* are listed in Table 3-1.

Table 3-1 Guidelines for interpreting the relative error *R* [10]

Range of R	Quality of the Tally
0.5 to 1.0	Not meaningful
0.2 to 0.5	Factor of a few
0.1 to 0.2	Questionable
< 0.10	Generally reliable
< 0.05	Generally reliable for point detectors

For all tallies, except for the point detector tallies, also referred to as next-event tallies, the relative error should be less than 0.10. For a well-behaved tally, *R* will be proportional to 1/sqrt(N). Thus, to halve *R*, the total number of histories must fourfold. But this could lead to very long computation times, for example to reduce *R* by a factor of 10, the computation time should be a hundred times longer. Therefore MCNP has special variance reduction techniques to decrease *R*, without increasing hardly any computation time.

III. Variance reduction

Variance reduction techniques is something I have not used during this thesis, but what I want to mention, since it's of good use for reducing the relative error and the computation time, because one of the difficulties with the MC method is the need for large computational time *T*. Since *T* consumed is proportional to *N*, and *R* is proportional to *1/sqrt(N)*, *R = C/sqrt(T)*, where *C* is a positive constant [10]. In MCNP5 manual volume I [10] the special techniques are given to decrease *C*.

3.3. Optimization

3.3.1. Introduction

Since we now have a working MCNP script we can design a script which can find a maximum for the goal function, which is defined later on in this section. In Figure 3-4 a schematic is given of how the optimization script looks like. In here *Filter.i* and *Filter.out* are both MCNP files, where *.i* stands for input and *.out* for output file respectively. This means that the script should be able to read and write MCNP output and input files, so that the optimization code can find a maximum. Therefore the optimization code, or method, used in this thesis will be discussed in the next section, where after the whole script, written in Perl, will be discussed.

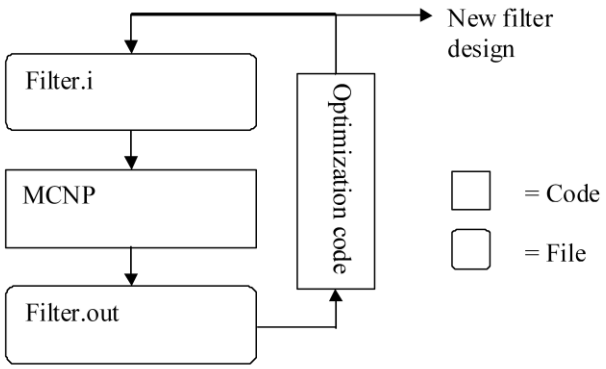

Figure 3-4 **A schematic of the optimization script used to find a new filter design. The two blocks with curved angles are MCNP input and output files respectively. The blocks with sharp angles is code, i.e. the MCNP program and the optimization script.**

3.3.2. Optimization method

I. Gradient ascent method

The gradient descent method is a very useful method for finding a local minimum, or when searching for a local maximum, it's called the gradient ascent method. From now on I will call it the gradient ascent method, because I presume that we will search for a maximum.

The gradient ascent method is based on the principle that any at least one differentiable real-valued function $DF(\boldsymbol{d})$ increases most in the positive direction of its gradient. This could be done in n dimensions and is represented by:

$$\begin{pmatrix} d_{1,i+1} \\ d_{2,i+1} \\ \vdots \\ d_{n,i+1} \end{pmatrix} = \begin{pmatrix} d_{1,i} \\ d_{2,i} \\ \vdots \\ d_{n,i} \end{pmatrix} + \gamma \vec{\nabla} DF \begin{pmatrix} d_{1,i} \\ d_{2,i} \\ \vdots \\ d_{n,i} \end{pmatrix}, \tag{3.4}$$

where the vector $\boldsymbol{d}_{i+1}$ represents the new coordinates and $\boldsymbol{d}_i$ represents the old coordinates, γ is just a constant to determine the increments between the old and new coordinates.

In Figure 3-5 an example of a curved landscape is shown. The gradient ascent method could be used for finding a local maximum, but be aware of the fact that the maximum you find depends on the starting position. This picture could be an example of the goal function determined by measuring its value by investigating two different types of filter/ moderator materials. If more materials are investigated such pictures can not be made.

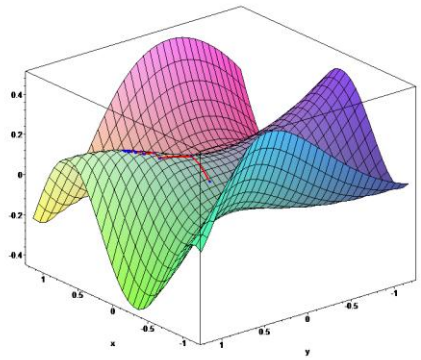

Figure 3-5 **An example of curved landscape in which local maxima could be found by using the gradient ascent method. Note that the maximum you find depends on the starting position. The values on the x- and y-axis could be a thickness of two different types of materials. The z-axis could be the value of the goal function. www.wikipedia.org**

II. Goal function

The function which is being optimized by the gradient ascent method is called the goal function. Since I want the goal function to increase if the *epithermal* neutron current increases or the *thermal* or *fast* neutron current decreases, the following function satisfies these conditions[18]:

$$DF = \frac{\phi_{epi}}{\phi_{ther} + \phi_{fast}}. \tag{3.5}$$

The relative error of the goal function is given by[19]:

$$\frac{u(DF)}{DF} = \frac{1}{\phi_{ther} + \phi_{fast}} u(\phi_{epi}) - \frac{\phi_{epi}}{(\phi_{ther} + \phi_{fast})^2} u(\phi_{epi}) - \frac{\phi_{epi}}{(\phi_{ther} + \phi_{fast})^2} u(\phi_{fast}) \tag{3.6}$$

3.3.3. Perl

The Perl script is written to find the best thickness for two different materials, but could increase the number of materials by just adding more subroutines. In Appendix C. Perl script the Perl script is given. In Appendix C1. Perl script in blocks the Perl script is given within blocks, which is handy to refer to and in Appendix C2. Perl script the Perl script is just given without those blocks.

The parameters used for the optimization are defined in block 1. Also some results, such as neutron current and thicknesses of materials must be stored during the optimization run. These data will be stored in arrays, which are also defined in block one. Arrays are defined by an @, where scalars are defined by an *$*.

The optimization is done by using a while loop and is defined in block two. When the precision is bigger than a certain number, the optimum has not been found and the loop

---

[18] This was my first goal function. Later on the goal function is defined as: $DF = \frac{\phi_{epi}}{\phi_{total}}$.

[19] The relative error of a function $f(x, y)$ is given by: $\frac{u(f)}{f} = \frac{\partial f}{\partial x} u(x) + \frac{\partial f}{\partial y} u(y)$.

continues. The precision is defined as the sum of the absolute values of the gradient. In block two, the MCNP input file has also been made. In here, surfaces three, four and five are variable and only surfaces three and four can change due to the gradient ascent method, where surface five is only surface four plus a constant. After the MCNP input file has been made, it can be executed. This is done in block 3. The *wait* command is inserted to let the script wait till this MCNP file has been executed.

Now MCNP is running and after a certain amount of time an MCNP output file has been created. But since that time is not constant, but may increase if the filter thickness increases, in block 4a and 4b a loop is inserted. If the file does not exist it will be looped continuously[20], but because the file will be created some time[21], the loop will end and the MCNP output file will be read. Then in the first subroutine in block 4a the right data will be pulled out of the output file and is stored in an array (*@lines*). Each line contains three different types of data, first it contains the energy of the bin, secondly it contains the normalized neutron current and at last it contains the relative error. In Figure 3-6 part of the useful data of an MCNP output file is given to illustrate the three numbers on each line. Perl reads each line as one scalar, so that scalar must be cut in three parts to obtain the right data. That data 'splitting' will be done in the second subroutine.

```
1.0000E-04   2.44691E-03 0.0197
2.0000E-04   2.28034E-03 0.0205
3.0000E-04   1.82480E-03 0.0229
4.0000E-04   1.58396E-03 0.0246
5.0000E-04   1.37039E-03 0.0265
6.0000E-04   1.29429E-03 0.0272
7.0000E-04   1.17795E-03 0.0286
8.0000E-04   1.03784E-03 0.0304
9.0000E-04   1.01176E-03 0.0308
1.0000E-03   8.88638E-04 0.0329
2.0000E-03   7.11123E-03 0.0116
3.0000E-03   4.87098E-03 0.0140
4.0000E-03   3.81562E-03 0.0159
```

Figure 3-6 Part of the useful data of an MCNP output file.

In block 4b the data will be sorted and stored in an array. The goal function is also determined in this block.

In block five the difference in the goal function value will be measured using a for loop, where in block six the gradient will be determined. According to eq. (3.4) a gamma must be chosen to scale the (discrete) gradient. This is also done in block six. The precision seen earlier in block one will be determined in this block and is defined as the absolute value of the sum of both gradients. The precision indicates the increment between to point, i.e. the step size.

Finally in block seven, all data will be stored and printed to a file called GRASMETHDATA, which refers to GRadient AScent METHod DATA. When the run is finished the following sentence will be printed to the screen: *Run is finished, you can have coffee now!*

[20] When this loop runs, the computation time could increase. To reduce computation time, one could insert a *wait* command to wait for example ten seconds to run the loop again.

[21] There is a possibility that the MCNP output file will not be made, that happens in the case that there occurred a fatal error in the input file. But I presume that the MCNP input file will remain fatal error free, since the first MCNP input file is certainly 'good'.

3.4. Measuring method

In fact, there are three parameters in the filter/ moderator arrangement which can be optimized, that is: i) which materials are going to be used in the filter/ moderator arrangement; ii) the number of materials in the FM arrangement and iii) the thickness of the material layers. Since the goal function determines the optimal thickness of the material layers, I will choose the number and which materials are used in the FM arrangement. According to the discussion given in section 2.4 I will examine the following FM specifications.

3.4.1. FM I Determine current and goal function

First I want to measure the goal function in one dimension, i.e. only the thickness of one material layer will change. The goal function will be obtained with a slight change in the optimization script. Instead of determining the discrete derivative a command line is inserted to change the thickness with 0.1 cm en determine the goal function again. The goal function will be measured using the following materials:

- 10 cm Al_2O_3
- Variable carbon layer between 0.1 and 80.1 cm with increments of 0.1 cm
- 0.1 cm B-10

3.4.2. FM II First practice with optimization script

After this first practice the optimization script will be tested, using the same materials, but now taking the thickness of Al_2O_3 also variable. The starting points are:

- 5 cm Al_2O_3 (variable)
- 5 cm natural C (variable)
- 0.1 cm B-10 (constant)

Now it could be verified whether the script follows the same goal function line for the thickness of the carbon layer as found during the determination of the current and goal function in section 3.4.1.

The gradient will be determined by measuring the goal function as function of thickness for a thickness change of five per cent, therefore the denominator in eq. (3.4) will be *0.05*thickness*. The gamma in the gradient ascent method will be taken constant and has value of 50.

3.4.3. FM III Final run

As a final run of the optimization script the following materials will be used:

- 2 cm natural Fe (variable)
- 10 cm Ar-40 (variable)
- 1.5 cm Li-6 (constant)

Since Li-6 was 5 times less in absorbing neutrons and the density is approximately 3-4 times less than B-10 the thickness of the Li layer should be 15-20 times bigger than the B layer. Therefore I have chosen the Li layer to be 1.5 cm. At room temperature argon is in the gaseous phase, but since the atom density will be very low, I presume that the argon will be cooled to the liquid phase. The relative density of argon in the liquid phase is 1.4, the relative

density of water equals 1. I have chosen argon, because that is also be used in the FM arrangement in Petten.

4. Results

4.1. Introduction

In this chapter the results of some (test) runs of the script will be presented accompanied by intermediate conclusions to improve the optimization script.

4.2. Determination of current and goal function

4.2.1. Current and goal function

As a first test the neutron current in the three energy regions were measured with a varying thickness of carbon layer. The FM arrangement was as follows: 10 cm Al_2O_3, 0.1-80.1 cm with increments of 0.1cm C and 0.1 B-10. The results are given in Figure 4-1. Here it can be seen that the epithermal neutron current has its highest value at around 10 cm of carbon layer.

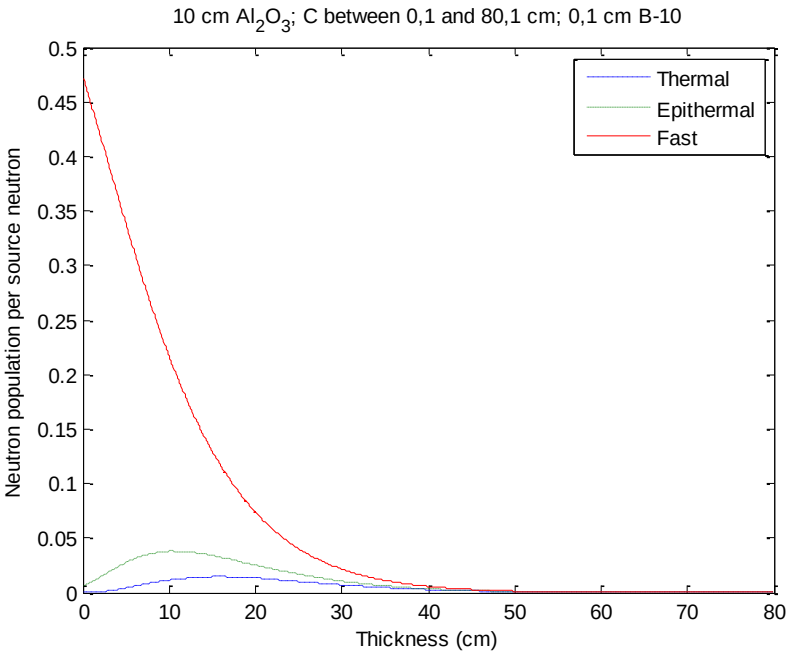

Figure 4-1 **The thermal, epithermal and fast neutron current for a variable thickness of carbon layer in a FM arrangement with 10 cm Al_2O_3 and 0.1 cm B-10. The thickness of carbon varies between 0.1 and 80.1 cm, with increments of 0.1 cm. At 10cm the epithermal neutron current has its highest value and after approximately 40 cm, all neutrons are absorbed.**

In Figure 4-2 the ratio between the epithermal and thermal plus fast neutron current (Eq. (3.5)) is given. We saw in Figure 4-1 that the epithermal flux has its highest value at 10cm, but the goal function[22] has its highest value at approximately 38 cm. This could be ascribed to the fact that the fast neutron current is still very high at 10cm, but decreases rapidly.

After a thickness of 10cm the total neutron current is approximately zero, which also can be seen in Figure 4-2. The sharp peaks in that figure indicate a high uncertainty and a relative error in the range of 0.5-1, which is not meaningful (Table 3-1).

[22] In this goal function, the epithermal neutron current was in the energy region of 1 keV to 20 keV. The thermal neutron current was below 1 keV and the fast neutron current were all neutrons above 20 keV.

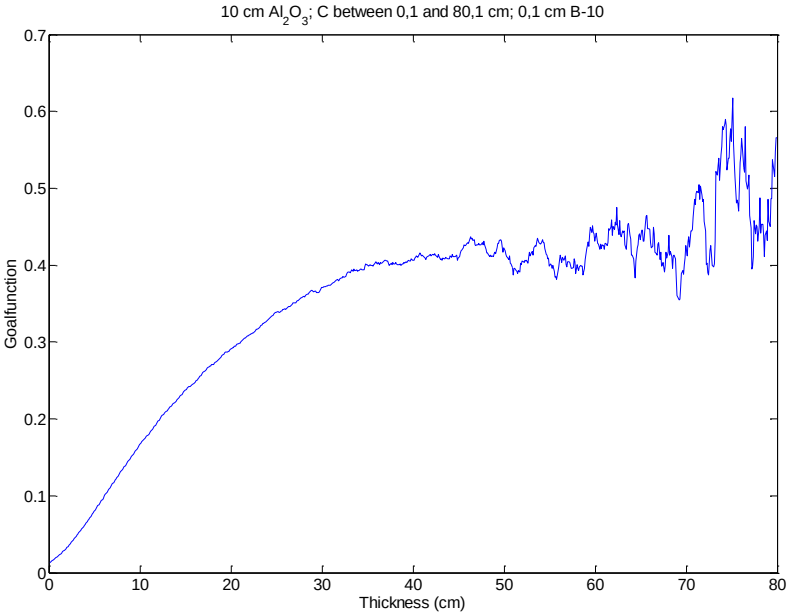

Figure 4-2 **Goal function of the FM arrangement given in Figure 4-1. The epithermal neutron current was in the energy region of 1-20 keV, the thermal neutron current was below 1 keV and the fast neutron current were all neutrons above 20 keV.**

4.2.2. Conclusion

From this test it can be seen that the epithermal neutron current is still very low, but this could be clarified by the fact that the neutron source is mono-energetic with energy of 2 MeV. Therefore, it could be better to introduce a more realistic neutron source, but since that won't influence the optimization code I have not done that and kept the neutron source unchanged.

What also can be seen, mainly in Figure 4-2, is that when the neutron population becomes too low, the uncertainty increases. Therefore, a new parameter may be introduced in the script that when the neutron population decreases, the number of neutrons tracked must increase, i.e. the number behind the NPS command in MCNP must increase (see section 3.2.3).

In simulation there will be made some assumptions to reduce computation time. Therefore, the neutrons won't be simulated one to one and the criteria given in section 1.4.1, that the epithermal neutron intensity should not be less than 10^9 n_{epi} cm^{-2} s^{-1}, can not be satisfied. Therefore I have inserted another criterion in the optimization script. According to Figure 4-1, the epithermal neutron flux should not be less then 0.01, or 1 per cent of the total source neutron current, to give accurate results. I have also made a slight change in the goal function given in eq. (3.5). Instead of only dividing by the *thermal* and *fast* neutron current, the *epithermal* neutron current will be divided by the total neutron current.

4.3. First practice with optimization script

4.3.1. Results from first practice

In Table 4-1 the results from this first run are given. In here *D1* and *D2* are thicknesses of material one and two, respectively Al_2O_3 layer and C. The goal function is measured as the *epithermal* current divided by the total neutron current.

Table 4-1 Results from first practice with optimization script. Note that the change in thickness for both materials is not constant. This script was terminated after the third cycle, since the fourth thicknesses for both materials absorbed too much neutrons, which results in an *epithermal* neutron current less than 1 per cent of the neutron source. The uncertainty of the *thermal*, *epithermal* and *fast* neutron current given in the MCNP output are given by u(ther), u(epi) and u(fast) respectively. DeltaD1 and DeltaD2 refer to the change in thickness of material one and two. The precision is just the sum of those two step sizes.

Script Run	1	2	3	4
D1 (cm)	5	5.5789	15.8336	45.9380
D2 (cm)	5	5.7835	15.9766	45.5417
Goal function	0.0331	0.0534	0.4638	-
Φ_{Ther}	0.00	1.9710E-06	1.8296E-05	0.00
Φ_{Epir}	1.5089E-02	2.2900E-02	2.4591E-02	2.9973E-06
Φ_{Fast}	4.5597E-01	4.0630E-01	2.8433E-02	0.00
σ (Φ_{Ther})	0	0.7071	0.2309	0.00
σ (Φ_{Epir})	0.0079	0.0064	0.0062	0.5773
σ (Φ_{Fast})	0.0011	0.0012	0.0058	0.00
δ_{D1} (cm)	0.5789	10.2547	30.1044	Run terminated
δ_{D2} (cm)	0.7835	10.1931	29.5651	Run terminated
Precision	1.3624	20.4478	59.6695	Run terminated

4.3.2. Conclusion

The step sizes to new thicknesses of material one and to are respectively δ_{D1} and δ_{D2}. What can be seen from Table 4-1 is that these increments increase rapidly. Therefore this filter/ moderator arrangement will be run again, but with a variable gamma in the gradient ascent method (eq. (3.4)).

If the goal function increases, you will come closer to a (local) maximum (if there is any). Near a local maximum, the step size must decrease, and therefore gamma could be taken as the inverse of the goal function.

Table 4-2 Goal function and the inverse of the goal function.

Run	1	2	3	4
Goal function	0.0320	0.05336	0.4636	-
1/Goal function	31.25	18.74	2.16	-

In Table 4-2 the inverse of the goal function is given. What can be seen from this is that the inverse is of the same order as the old (constant) gamma in the previous run, except for run three, but that is nearer to an optimum so in that range the step size must be smaller. Therefore the optimization script will be run for the same filter/ moderator arrangement again, but with gamma as the inverse of the goal function value.

4.3.3. Results with variable gamma

The results for the run with the variable gamma but the same FM set up as in the previous section are given in Table 4-3.

Table 4-3 Results for a run with a variable gamma. The neutron currents are given per source neutron.

Run	1	2	3	4	5
D1 (cm)	5	5.3614	9.4365	11.6576	13.4399
D2 (cm)	5	5.4892	9.5469	11.7418	13.5057
Goal function	0.0320	0.0444	0.2187	0.3828	0.4335
Φ_{Ther}	0.00	9.8840E-07	1.7844E-05	1.7853E-05	1.3402E-05
Φ_{Epi}	1.50889E-02	1.97570E-02	5.03714E-02	4.62991E-02	3.75362E-02
Φ_{Fast}	4.55966E-01	4.24892E-01	1.79940E-01	1.00429E-01	6.05042E-02
σ (Φ_{Ther})	0	1.00	0.2357	0.2357	0.2696
σ (Φ_{Epi})	0.0079	0.0069	0.0043	0.0045	0.0050
σ (Φ_{Fast})	0.0011	0.0012	0.0021	0.0030	0.0039
δ_{D1} (cm)	0.3614	4.0750	2.2211	1.7822	1.5425
δ_{D2} (cm)	0.4891	4.0576	2.1948	1.7639	1.5196
Precision	0.8506	8.1326	4.4160	3.5462	3.0622
Γ	31.2186	22.5059	4.5726	3.1695	2.6122

Run	6	7	8	9
D1 (cm)	14.9824	16.3686	17.6265	18.7941
D2 (cm)	15.0253	16.3893	17.6291	18.7743
Goal function	0.4760	0.5097	0.5356	0.5357
Φ_{Thert}	1.2898E-05	1.6821E-05	1.3883E-05	1.1807E-05
Φ_{Epi}	2.9206E-02	2.2195E-02	1.6936E-02	1.2855E-02
Φ_{Fast}	3.8154E-02	2.4415E-02	1.6277E-02	1.1130E-02
σ (Φ_{Ther})	0.2719	0.2389	0.2673	0.2887
σ (Φ_{Epi})	0.0057	0.0066	0.0075	0.0087
σ (Φ_{Fast})	0.0050	0.0063	0.0077	0.0094
δ_{D1} (cm)	1.3862	1.2578	1.1675	1.0814
δ_{D2} (cm)	1.3639	1.2398	1.1452	1.0784
Precision	2.7501	2.4976	2.3127	2.1598
γ	2.3067	2.1007	1.9619	1.8667

4.3.4. Conclusion

For a constant gamma (50) the optimal thickness of the Al_2O_3 layer and the C layer are respectively 15.88 cm and 15.98 cm, the goal function is 0.46 and the *epithermal* neutron current is 2.46e-2 neutrons per source neutron. When the gamma is taken variable, the thickness of the Al_2O_3 layer and the C layer are respectively 18.79 cm and 18.77 cm, the goal function is 0.54 and the *epithermal* neutron current is 1.29e-2 neutrons per source neutron.

So a variable gamma defined as the inverse of the goal function gives runs with smaller step sizes, but results in a slightly different thickness, with less *epithermal* neutrons passing through the filter, but with a higher goal function value (which is the one being optimized). This means that this method gives a better result when we are taking the optimization of the goal function into account.

In the final test of the script the same definition for the variable gamma will be used, but applied to another FM set up.

4.4. Final run

4.4.1. First set up

As a final run the following FM set up has been tried:

- ?[23] cm SiO_2 (variable)
- ? cm natural Ar (variable)
- 1.5 cm Li-6 (constant)

First, two runs were done to see whether the epithermal neutron current is high enough (above a fraction of 0.01) for the start thicknesses of SiO_2 and Ar layers. This was not the case if the SiO_2 and Ar layer where both 5 cm thick (see Table 4-4). If the layers were respectively 5 cm for the SiO_2 layer and 75 cm for the Ar layer, the epithermal neutron current was still under the 0.01 (see Table 4-5).

Table 4-4 Neutron current for a FM set up of: 5 cm SiO_2, 5 cm Ar and 1.5 cm Li-6. The epithermal neutron current is under a value of 0.01 with respect to the number of source neutrons.

Φ_{Ther}	0.00000E+00 (0.0000)
Φ_{Epit}	3.80997E-04 (0.0496)
Φ_{Fast}	7.49712E-01 (0.0006)

The epithermal neutron current increases with a factor of ten (from 1e-4 to 1e-3), when the Ar layer increases with a factor of fifteen. So to increase the epithermal neutron current to the target value of 0.01, the layer should increase again by a factor of 15, which results in a thickness of 15^2 times bigger than the original thickness of 5 cm, i.e. 1125 cm. Therefore argon will not be tested in the final run[24].

Table 4-5 Neutron current for a FM set up of: 5 cm SiO_2, 75 cm Ar and 1.5 cm Li-6. The epithermal neutron current is still under a value of 0.01 with respect to the number of source neutrons.

Φ_{Ther}	0.00000E+00 (0.0000)
Φ_{Epit}	1.00877E-03 (0.0293)
Φ_{Fast}	4.34042E-01 (0.0011)

4.4.2. Second set up

Now, Ar has been replaced by C, so that only SiO_2 and Li-6 will be different according to the first test with the script. With the following start parameters, the epithermal neutron current is above 0.01 with respect to the number of source neutrons:

- 15 cm SiO_2 (variable)
- 15 cm natural C (variable)
- 1.5 cm Li-6 (constant)

4.4.3. Results

With the start conditions given in the previous subsection the *epithermal* neutron current is 1.03e-1 and gamma has a value of 3.70. But the precision is smaller than 0.01 (see Table 4-6), which means that, according to the definition of the while loop, the search for a maximum has

[23] The question mark indicates that the thicknesses were not yet determined for which the *epithermal* neutron current is above 0.01.

[24] Ar is being used in the High Flux Reactor in Petten to moderate the neutrons. Therefore, we can not conclude from this single run that Ar is a poor moderator. Only is this setting, Ar isn't good enough.

been terminated. When the start thicknesses are 10 cm and 15 cm for respectively SiO_2 and C, the precision is bigger than 0.01 and a second run will start.

Table 4-6 Certain parameters for different staring thicknesses for the SiO_2- and C layer. If the precision is smaller than 0.01, the run is terminated. This is the case in which the start thicknesses are both 15cm or 18cm. When the starting thicknesses are respectively 10cm for the SiO_2- and 15cm for the C layer, the condition for the precision is satisfied, and a second run will be started.

D1/ D2 (cm)	Goal function	Φ_{Ther} (σ (Φ_{Ther}))	Φ_{Epi} (σ (Φ_{Epi}))	Φ_{Fast} (σ (Φ_{Fast}))	γ	δ_{D1} (cm)	δ_{D2} (cm)	Precision
15/ 15	0.27	2.99-06 (0.5774)	3.84E-02 (0.0049)	1.04E-01 (0.0029)	3.70	0.0353	0.0631	0.0985
18/ 18	0.35	5.99E-06 (0.4082)	2.82E-02 (0.0058)	5.34E-02 (0.0041)	2.89	0.0203	0.0377	0.0580
10/ 15	0.23	3.99E-06 0.5000	4.21E-02 0.0047	1.43E-01 0.0024	4.39	0.0316	0.0823	0.1139

The results of the run with the following FM set up and start thicknesses:

- 10 cm SiO_2 (variable)
- 15 cm natural C (variable)
- 1.5 cm Li-6 (constant)

are given in Table 4-7.

Table 4-7 Results of the run with a variable gamma and the following start thicknesses: 10 cm SiO_2, 15 cm C and 1.5 cm Li-6. Only the SiO_2- and C layer are taken variable.

Run	1	2	3	4
D1 (cm)	10	10.0316	10.0623	10.0903
D2 (cm)	15	15.0823	15.1640	15.2416
Goal function	0.2275	0.2294	0.2316	0.2334
Φ_{Thert}	3.9952E-06	3.9952E-06	3.9952E-06	3.9952E-06
Φ_{Epi}	4.2120E-02	4.1993E-02	4.1972E-02	4.1872E-02
Φ_{Fast}	1.4300E-01	1.4109E-01	1.3928E-01	1.3756E-01
σ (Φ_{Ther})	0.5000	0.5000	0.5000	0.5000
σ (Φ_{Epi})	0.0047	0.0047	0.0047	0.0047
σ (Φ_{Fast})	0.0024	0.0024	0.0024	0.0024
δ_{D1} (cm)	0.0316	0.0307	0.0280	0.0300
δ_{D2} (cm)	0.0823	0.0817	0.0776	0.0756
Precision	0.1143	0.1124	0.1056	0.1056
γ	4.3950	4.3598	4.3184	4.2854

Run	5	6	7	8	9
D1 (cm)	10.1203	10.1514	10.1850	10.2176	10.2515
D2 (cm)	15.3172	15.3939	15.47020	15.5473	15.6255
Goal function	0.2348	0.2366	0.2380	0.2393	0.24102
Φ_{Thert}	3.9951E-06	3.9951E-06	3.9951E-06	4.9942E-06	5.9934E-06
Φ_{Epi}	4.1715E-02	4.1576E-02	4.1416E-02	4.1200E-02	4.1057E-02
Φ_{Fast}	1.3589E-01	1.3413E-01	1.3257E-01	1.3090E-01	1.2928E-01
σ (Φ_{Ther})	0.5000	0.5000	0.5000	0.4472	0.4082
σ (Φ_{Epi})	0.0047	0.0047	0.0047	0.0047	0.0047
σ (Φ_{Fast})	0.0025	0.0025	0.0025	0.0025	0.0025
δ_{D1} (cm)	0.0311	0.0335	0.0326	0.0338	0.0338
δ_{D2} (cm)	0.0767	0.0762	0.0771	0.0781	0.0794
Precision	0.1078	0.1098	0.1098	0.1120	0.1132
γ	4.2576	4.2262	4.2011	4.1773	4.1489

Run	10	11	12	13	14
D1 (cm)	10.2853	10.3202	10.35341	0.3858	10.4187
D2 (cm)	15.7050	15.7820	15.8585	15.9325	16.0041
Goal function	0.2427	0.2448	0.2466	0.2482	0.2496
Φ_{Thert}	4.9955E-06	4.9955E-06	5.9947E-06	4.9957E-06	5.9810E-06
Φ_{Epi}	4.0909E-02	4.0816E-02	4.0684E-02	4.0517E-02	4.0373E-02
Φ_{Fast}	1.2760E-01	1.2585E-01	1.2425E-01	1.2268E-01	1.2132E-01
σ (Φ_{Ther})	0.4472	0.4472	0.4082	0.4472	0.4083
σ (Φ_{Epi})	0.0047	0.0047	0.0048	0.0048	0.0048
σ (Φ_{Fast})	0.0026	0.0026	0.0026	0.0026	0.0026
δ_{D1} (cm)	0.0348	0.0332	0.0323	0.0329	0.0343
δ_{D2} (cm)	0.0770	0.0764	0.0740	0.0716	0.0706
Precision	0.1118	0.1096	0.1063	0.1045	0.1049
γ	4.1192	4.0834	4.0543	4.0281	4.0052

4.4.4. Conclusion

The start conditions, i.e. the start thicknesses, were all ready near a local maximum, since the change of the goal function is very small. The change in thickness (δ_{D1} and δ_{D2}) is very small, but nearly constant. This fourteen runs, i.e. fourteen times three MCNP simulations took six hours of computation time.

5. Conclusions and Recommendations

5.1. Introduction

The main goal of this thesis was to write a script to optimize a certain goal function. That goal function is an indication of the quality of the FM set up, defined as the *epithermal* neutron current divided by the total neutron current. The optimization was done by using the gradient ascent method. This chapter gives the conclusions and some recommendations for further research.

5.2. Conclusions

Since the main goal of this thesis was to write a script and to demonstrate the method, the only results are in fact some test runs whether the script works and aren't in fact a representation of reality, since only the one dimensional case was taken into account with a mono-energetic neutron source. Although, there are some things that can be concluded from these test runs.

1. A maximum in the goal function defined in Eq. (3.5), and later on in this report defined as the *epithermal* neutron current divided by the total neutron current, doesn't mean that there is a maximum in the *epithermal* neutron current.
2. If the FM set up thickness increases, fewer neutrons will pass and the standard deviation (in measuring the neutrons) will increase, therefore insert a command that varies the number of histories tracked in MCNP, in order to obtain more accurate results from an MCNP run.
3. A variable gamma in the gradient ascent method gives a better controllable step size.
4. For the following FM specification: Al_2O_3 (variable thickness, start thickness of 5 cm), C (variable thickness, start thickness of 5 cm) and B-10 (constant 0.1 cm), the script finds, for a constant gamma of 50, a 'maximum' goal function value at 15.83 cm and 15.98 cm for respectively Al_2O_3 and C. The goal function value at that point is 0.46; the *epithermal* flux is 2.46e-2. For a variable gamma, defined as the inverse of the goal function, the thicknesses found for Al_2O_3 and C are 18,79 cm 18.77 cm. The goal function at that point is 0.54; the *epithermal* flux is 1.29e-2. Therefore, a variable gamma used in the gradient ascent method gives a better optimization of the goal function.
5. The run with a second FM specification, specified as follows: 10 cm SiO_2 (variable), 15 cm C (variable) and 1.5 cm Li-6 (constant), was terminated after a total of 42 runs, due to *runtpe* files which were all ready created in previous runs by MCNP. Therefore, to prevent this for next runs, a command must be inserted which deletes all unnecessary MCNP output files.

With this conclusions in mind, some recommendations can be made for further research.

5.3. Proceeding research

5.3.1. Goal function

In his thesis, Nievaart concluded that three neutron beams assure an optimal treatment, one nearly thermal (5 eV) and two epithermal (500 eV and 10 keV) [2]. Since my goal function does not take this into account a better goal function must be introduced to really obtain an ideal filter/ moderator arrangement.

In my thesis only the one dimensional case was taken into account. But to obtain a better result also the angle dependency of the neutrons which passes the FM set up must be measured. This is given as the *current-to-flux-ratio*. This could be a pre factor to scale the goal function, where a higher *current-to-flux-ratio* gives higher value of the goal function. In MCNP the angle dependency of the neutrons, or the direction in which the neutrons travel, can be measured by using a cosine card. This Cn cards works the same as the energy (En) cards, but now the energy bins are angle bins.

5.3.2. Optimization method

Mentioned earlier in chapter 3, one can optimize three parameters of the FM set up, i.e. the type of materials, number of materials and the thickness of materials. In fact one can optimize another parameter, namely the order in which the materials are placed in the FM arrangement. For this thesis I have only tried to optimize the thickness of the materials, but in fact, an optimization script should also be able to choose the number of materials and therefore which materials could be used in the FM arrangement. This is a very challenging assignment, but let me give a try.

Make a selection of materials and put those in one of three groups, type A, B or C, where: type A materials are all materials that could reduce the thermal neutron population (good absorbers in thermal region); type B materials are all materials that could reduce the fast neutron population (good scatterers in at least the fast energy range); and type C materials are all materials that could reduce the gamma ray contamination. This is something which could be done without using a computer by just looking at the cross section properties of materials and other properties defined in section 2.4.2. One can make a hierarchy in each group by just running simple MCNP files, now the optimization script ‘knows’ which materials are best in each group.

Since we now have different groups of materials the optimization script can be made to optimize the FM arrangement. Therefore we have to determine the total number of *thermal*, *epithermal* and *fast* neutrons and the change of *thermal*, *epithermal* and *fast* neutrons with respect to the last determination. When one of these numbers crosses a beforehand chosen number, the script tells us to insert a material of type A, B or C in the new input file to reduce the *thermal* or *fast* neutron population. When there is already such a material present in the input file, the script must only make that material thicker, but it could be possible that such a material is in fact not the right one to use, therefore a certain command must be inserted which can switch materials.

The change of the neutron population in the (three) different energy regions must be taken into account in the optimization method with respect to two successive runs, since an increase in (my) goal function could be due to a decrease in the total neutron current. This effect must be minimized, since that means that there are neutrons lost, which will decrease the efficiency of the FM set up and could lengthen the patients irradiation time.

This isn’t thé optimization method, and in fact this is very general, but it could be an anchor for writing an optimization script for this specific problem.

5.3.3. Computation time

In the preliminary design the computation time was in the order of hours, but in the optimizing method sketched above the computation time could increase to days or even

weeks. Surely when the FM set up will be optimized in three dimensions. Therefore, MCNP has something to reduce computation time, called Variance Reduction techniques. Else, neural networks can be used to train the script or even learn the script from several MCNP outcomes so that MCNP isn't in fact necessary anymore.

5.3.4. Neutron source

To obtain a more realistic outcome from MCNP a more realistic neutron source can be inserted, for example the one used at the High Flux Reactor in Petten.

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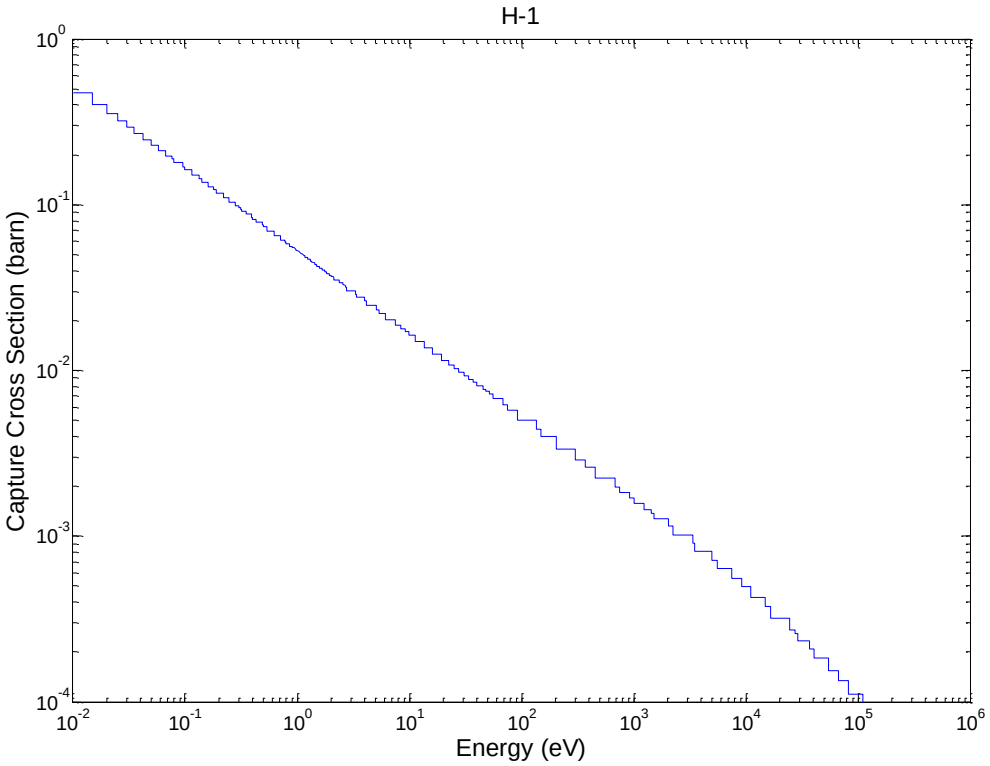
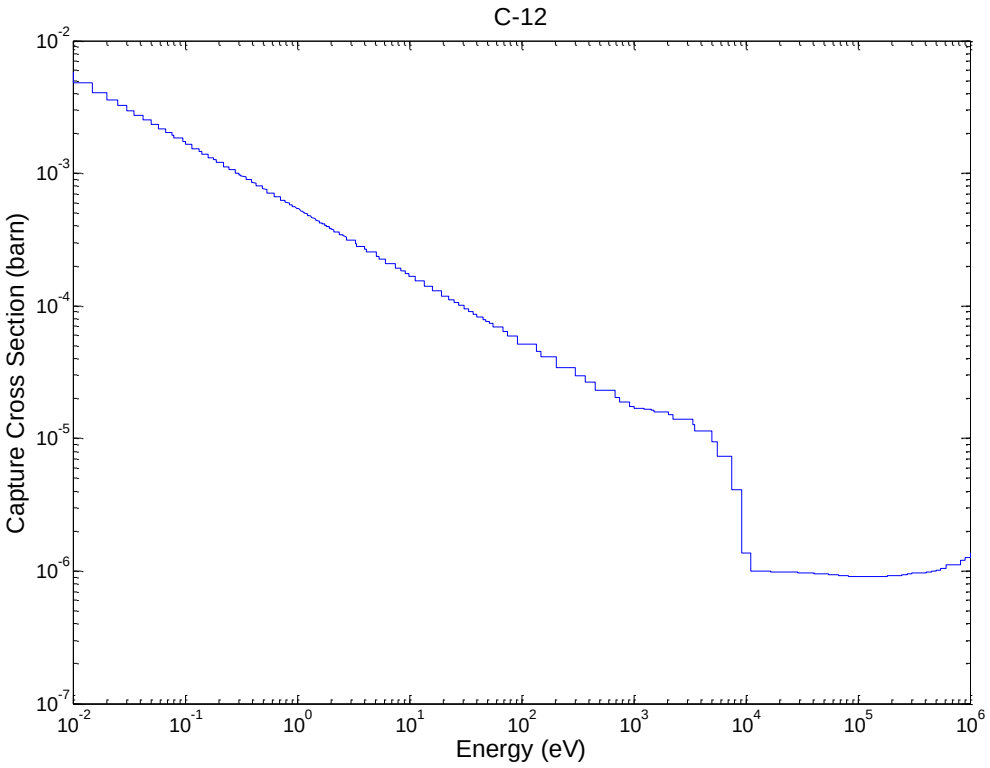
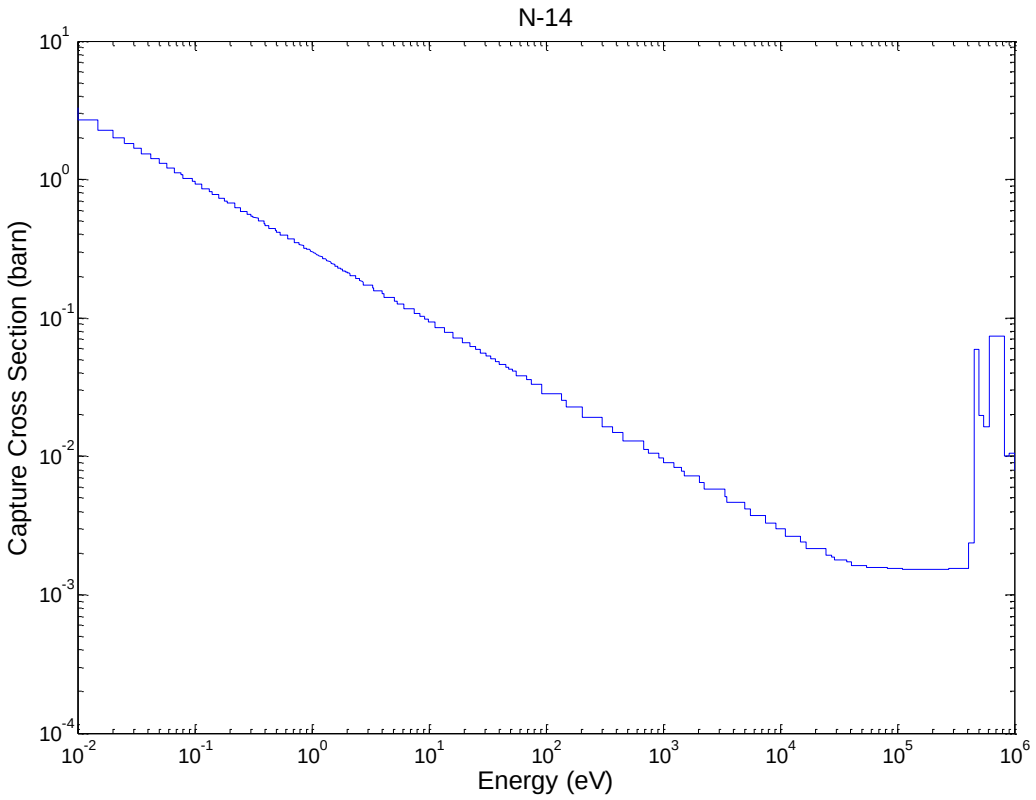
Appendix

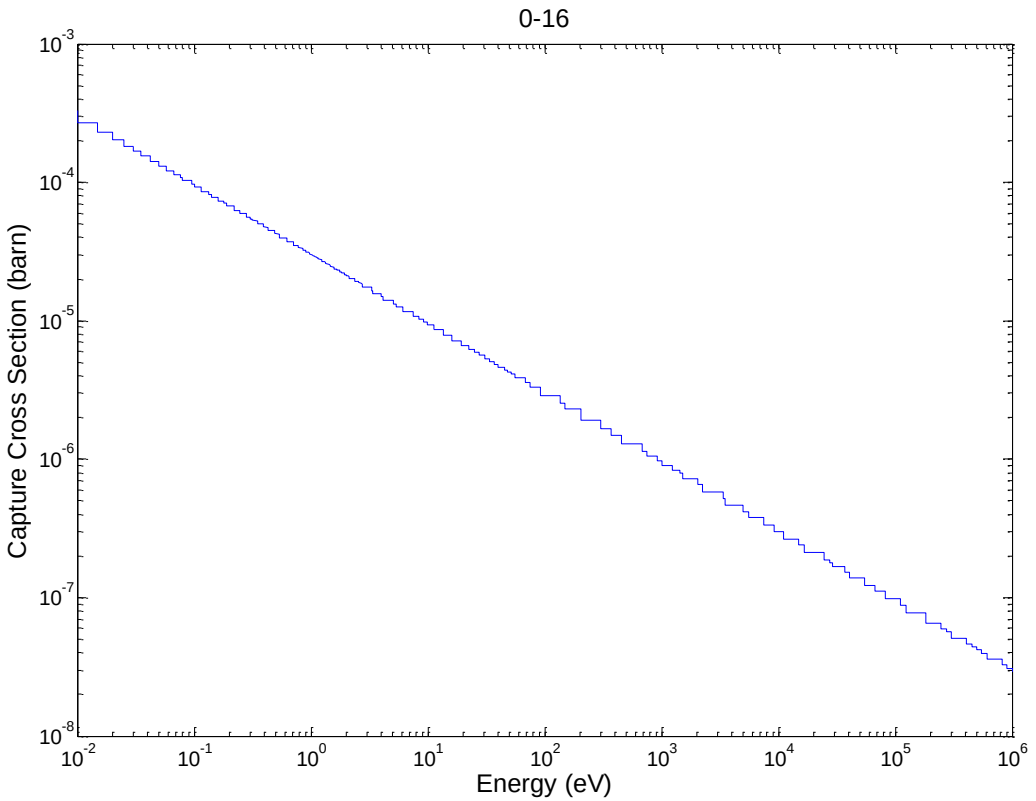
A. Cross sections plots

A1. Most common isotopes in human body

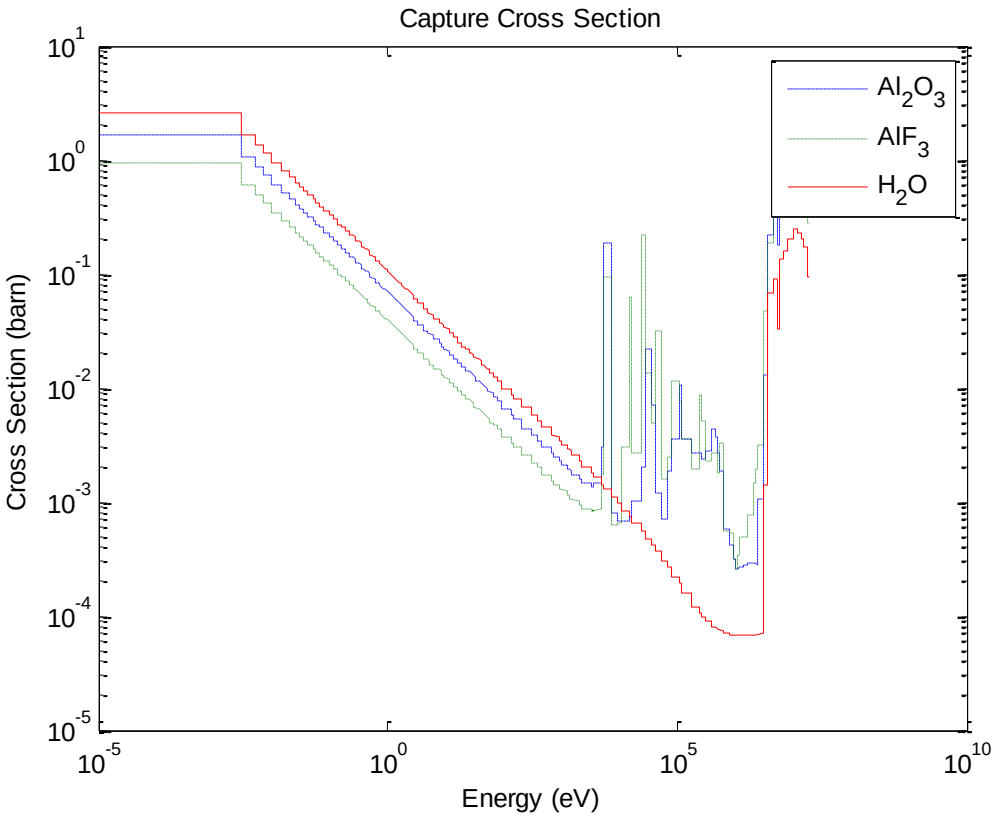


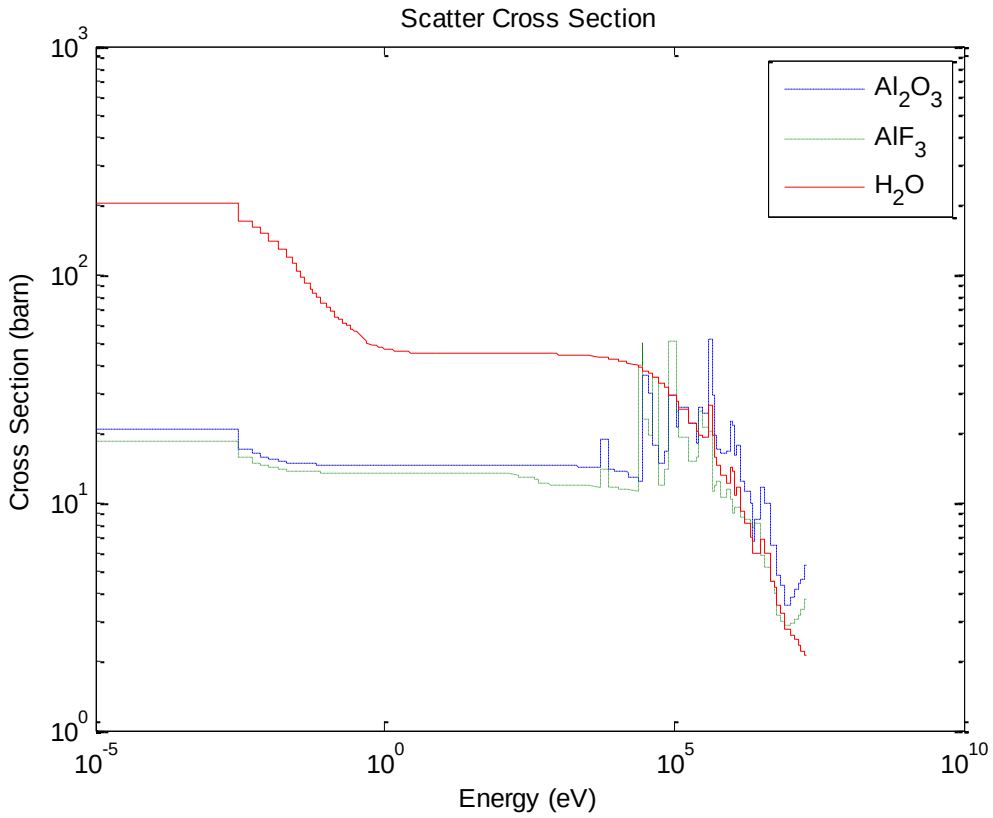



N-14
Capture Cross Section (barn)
Energy (eV)

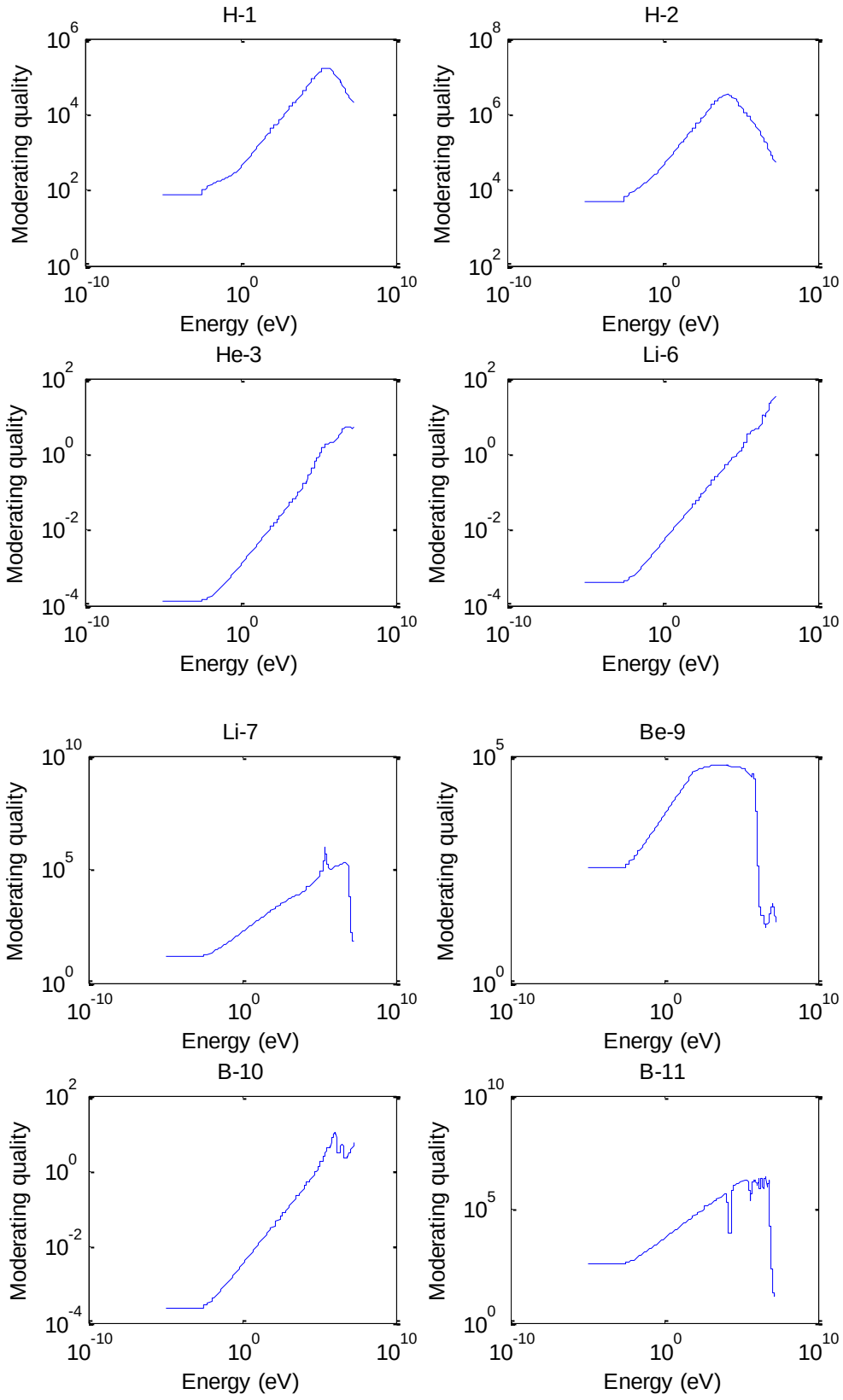

0-16
Capture Cross Section (barn)
Energy (eV)

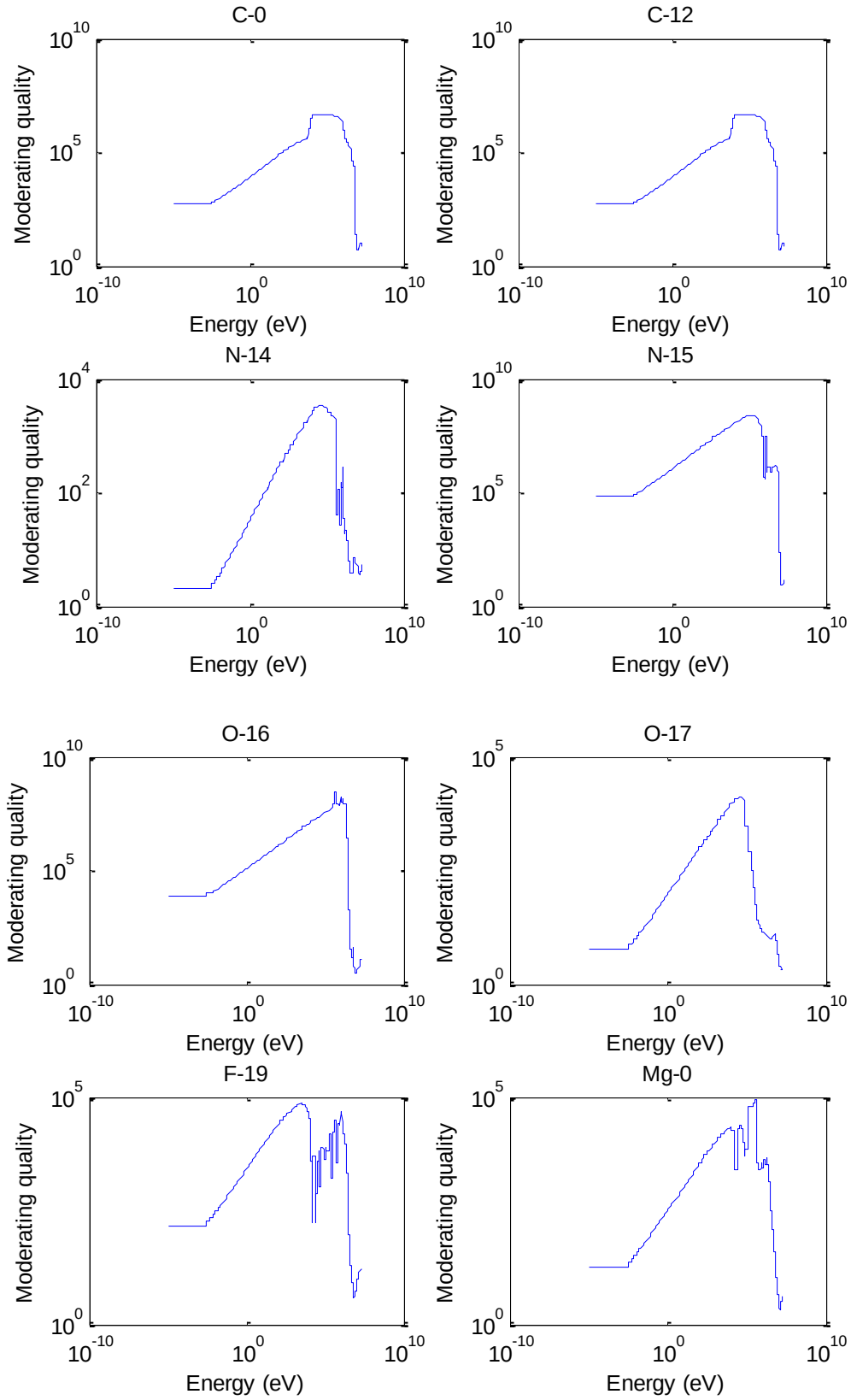
A2. Natural molecules





A3. Moderating quality isotopes

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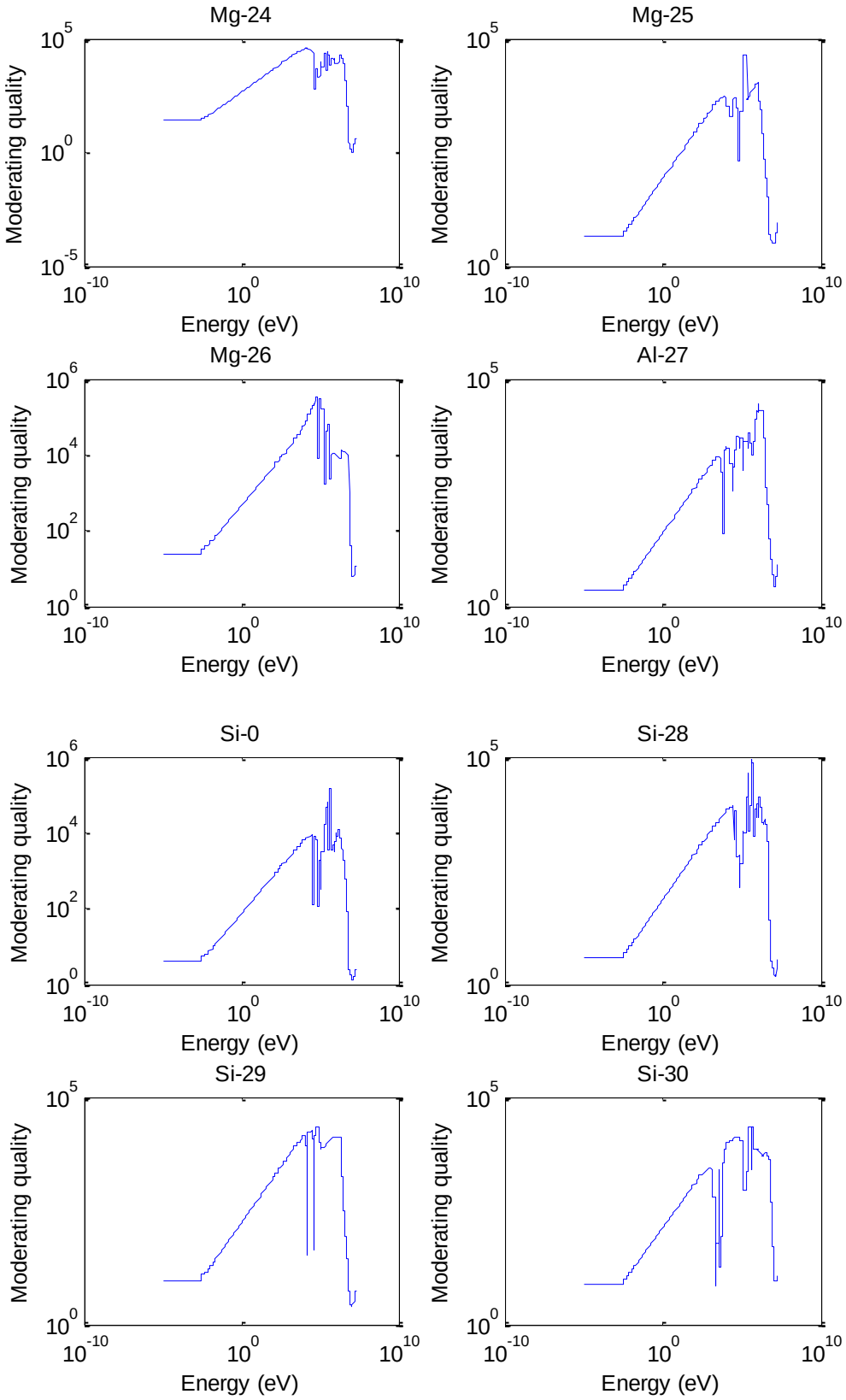
C-12
N-14
N-15
O-16
O-17
F-19
Mg-0
Moderating quality
Energy (eV)


Mg-24
Mg-25
Mg-26
Al-27
Si-0
Si-28
Si-29
Si-30
Moderating quality
Energy (eV)
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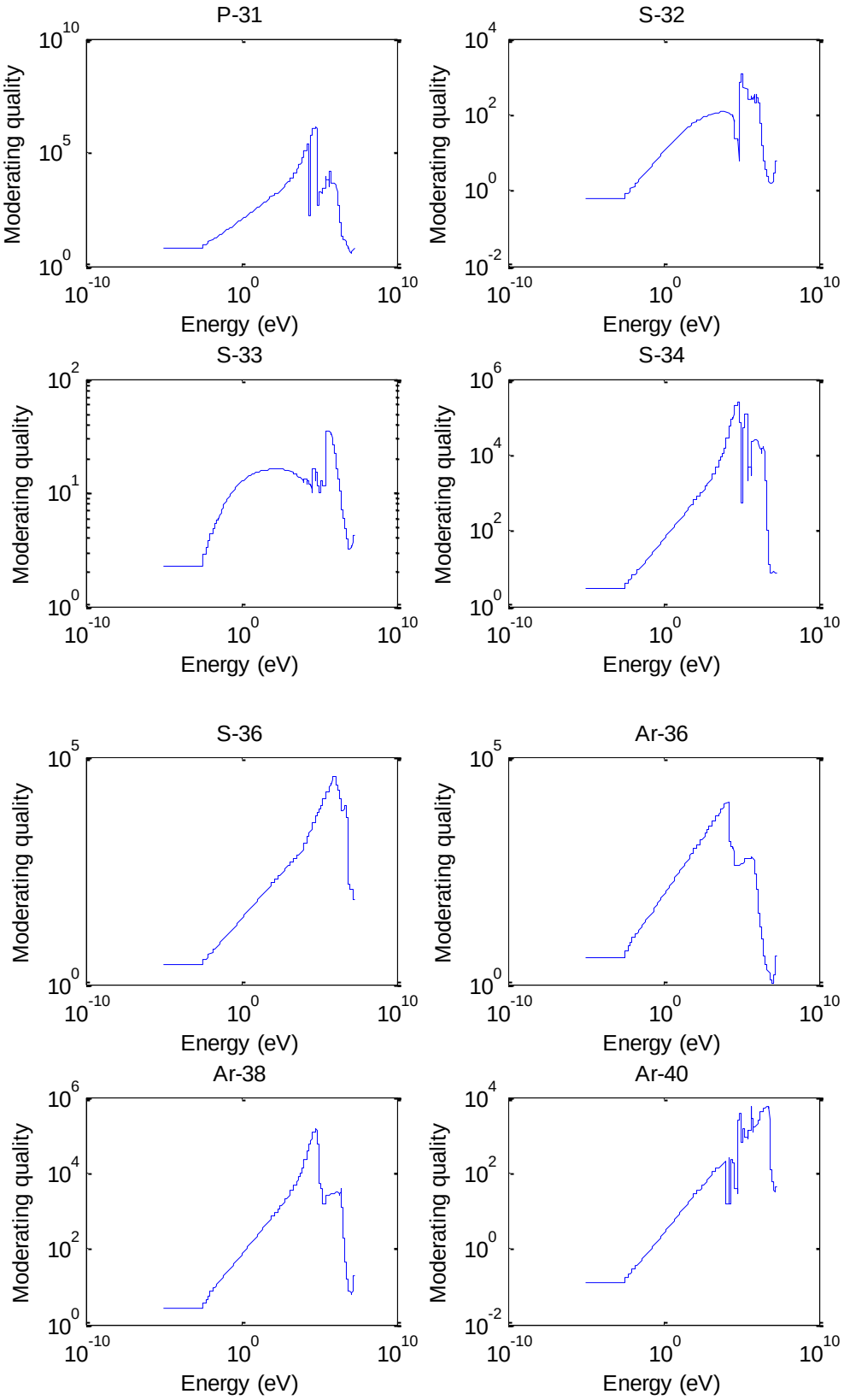
10^{5}
10^{0}
10^{2}
10^{4}
10^{6}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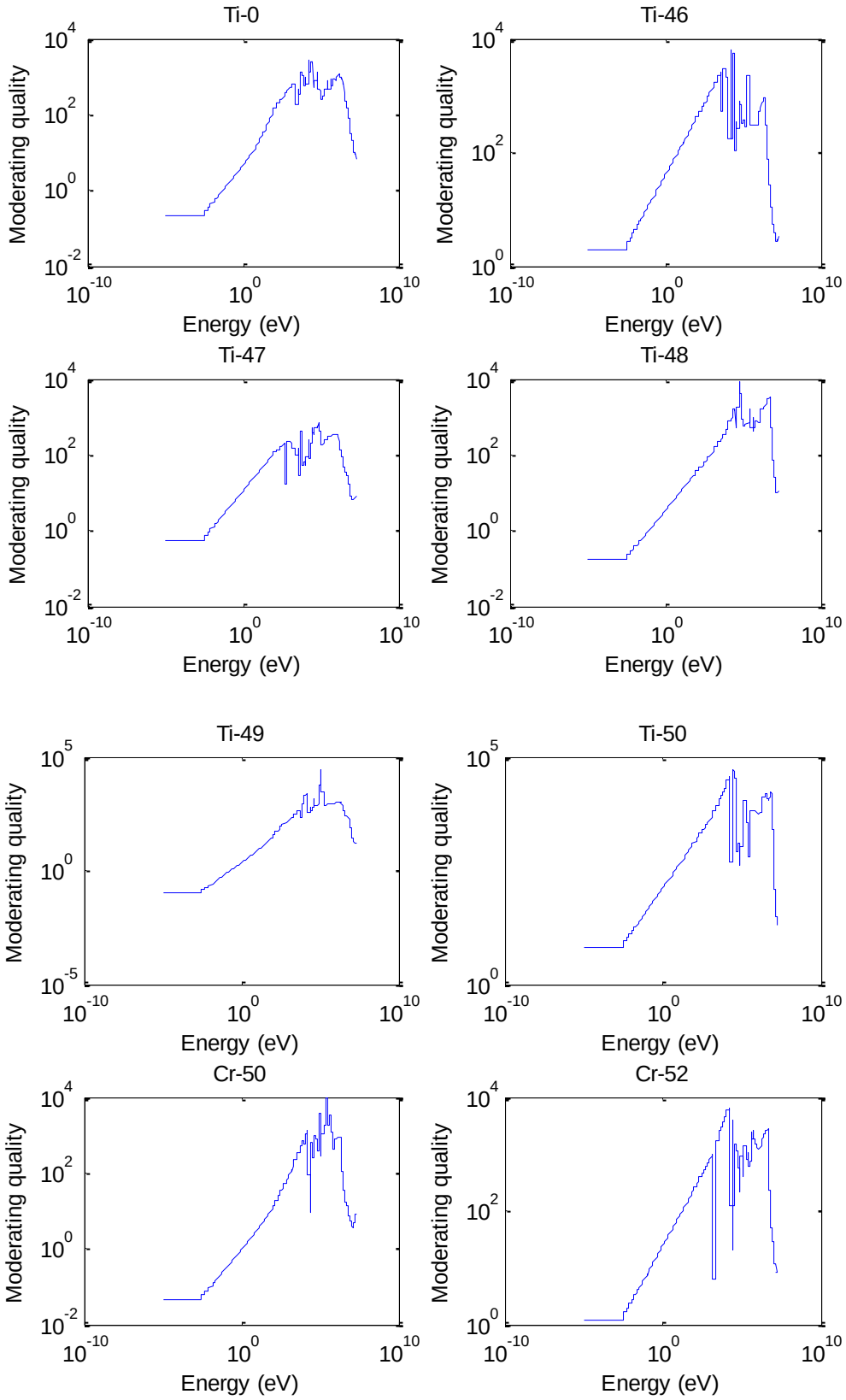
S-32
S-33
S-34
S-36
Ar-36
Ar-38
Ar-40
Moderating quality
Energy (eV)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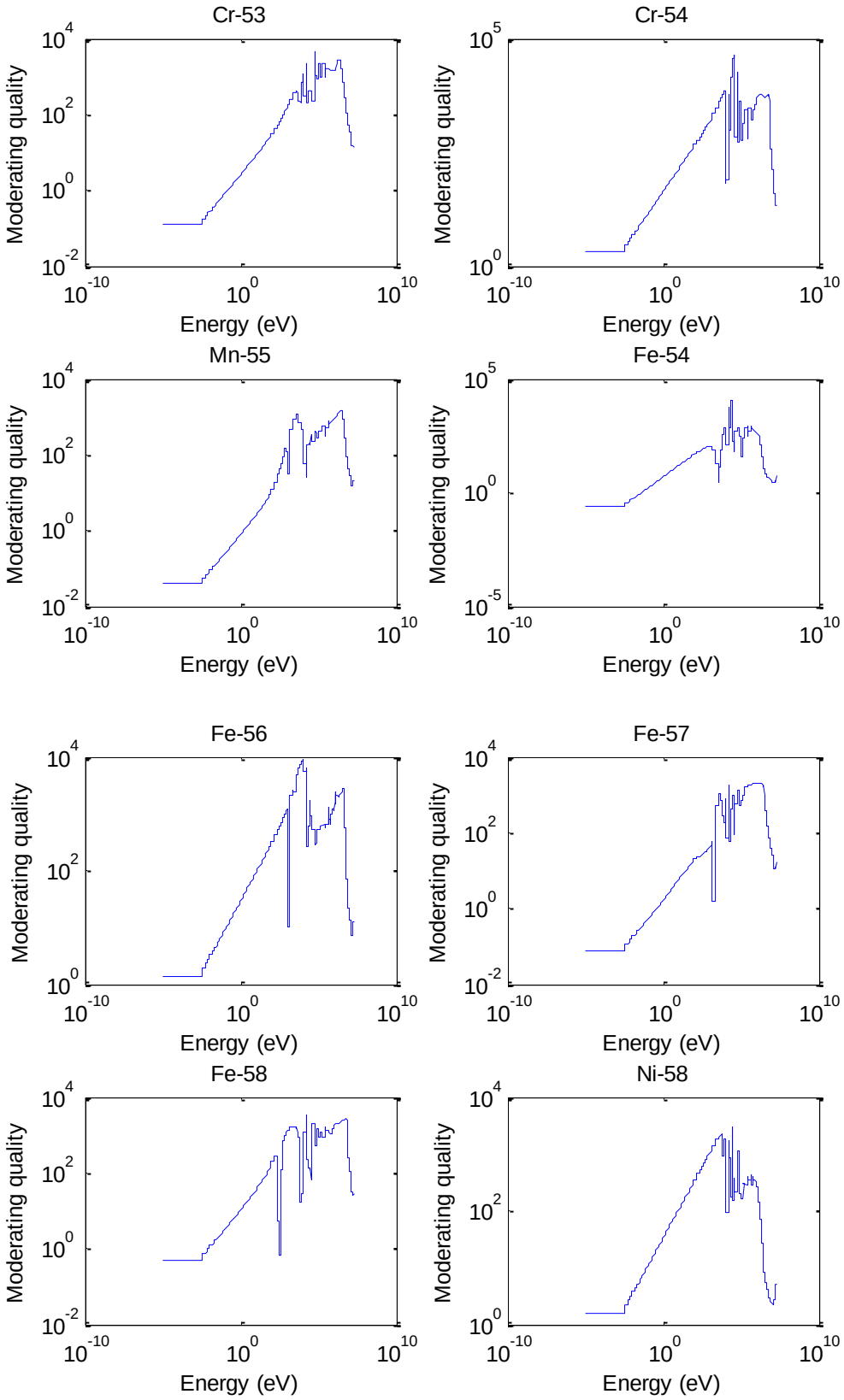
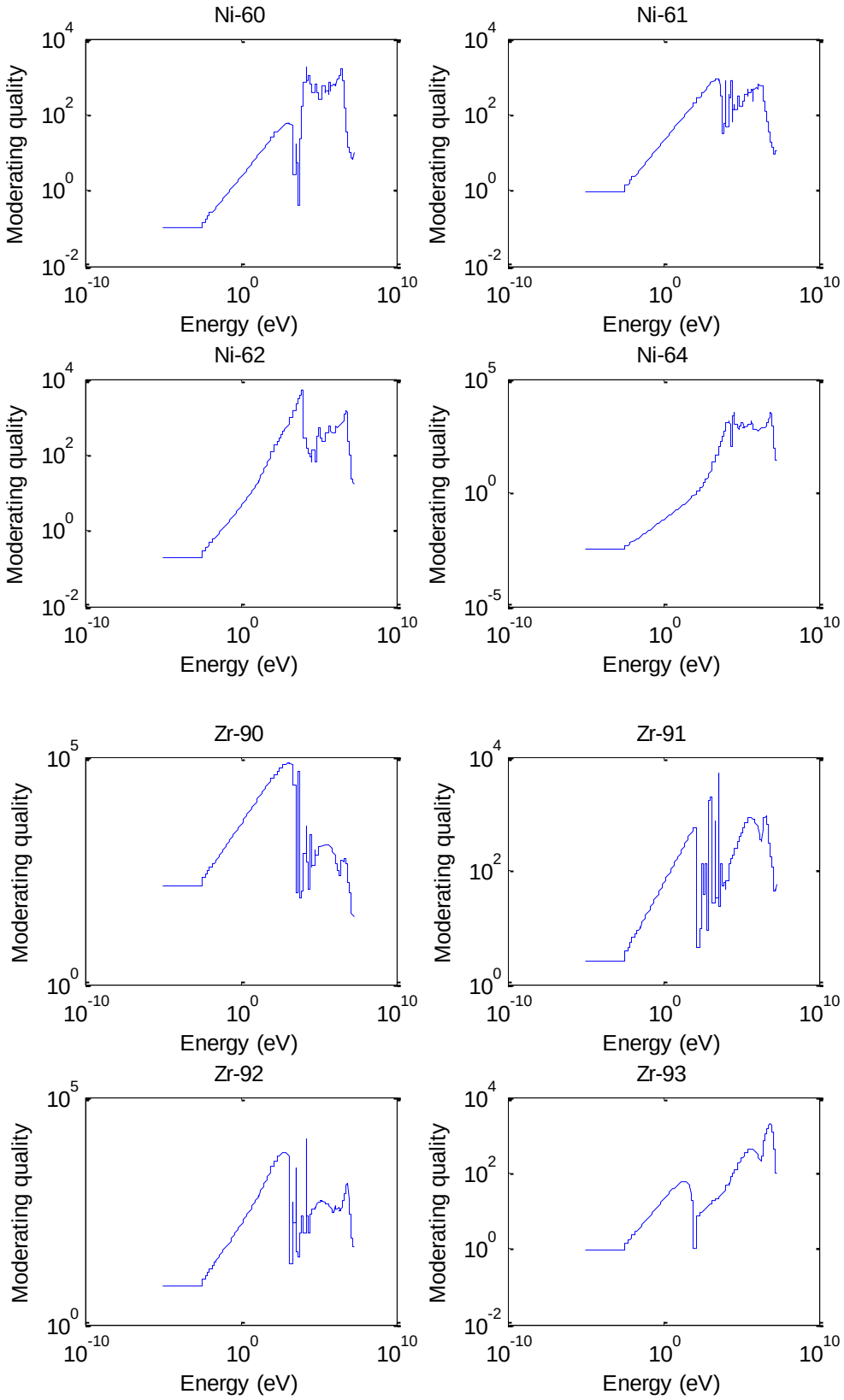
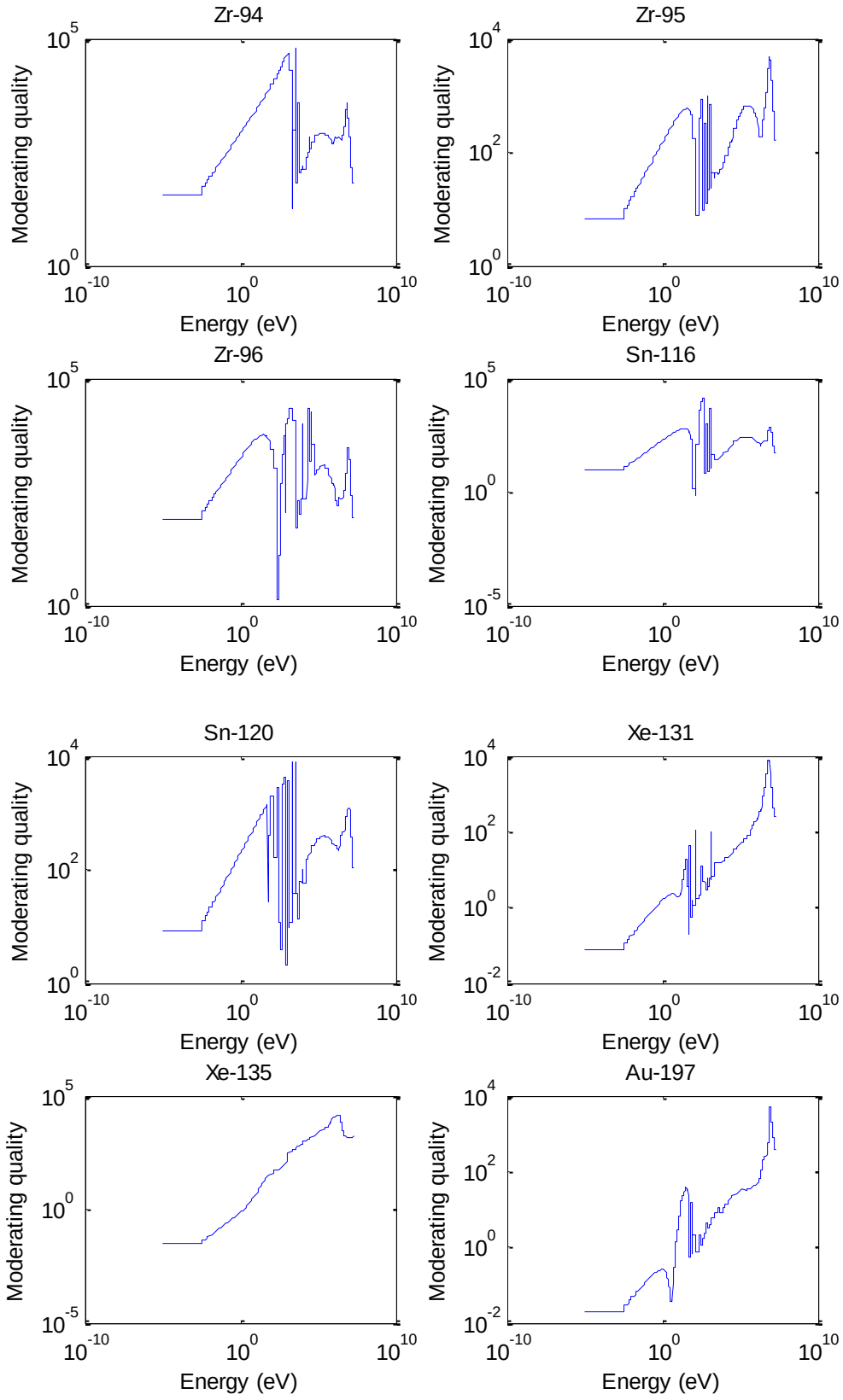
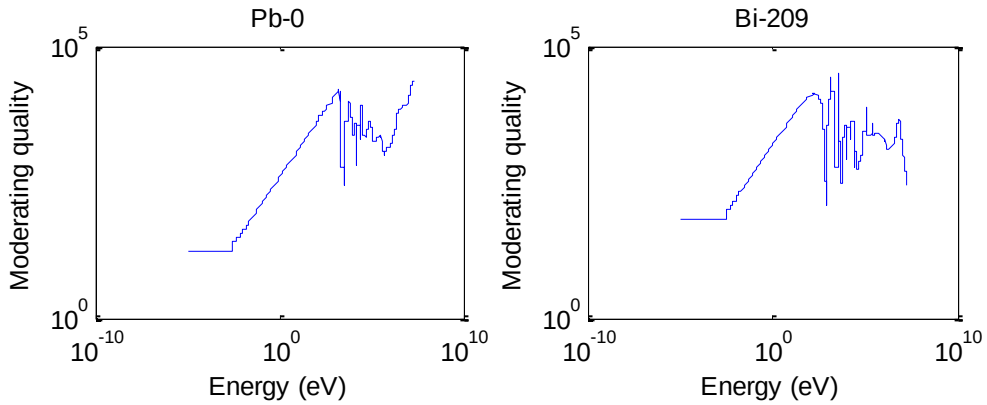
Ti-47
Ti-48
Ti-49
Ti-50
Cr-50
Cr-52
Moderating quality
Energy (eV)


Cr-53
Cr-54
Mn-55
Fe-54
Fe-56
Fe-57
Fe-58
Ni-58
Moderating quality
Energy (eV)


Ni-60
Ni-61
Ni-62
Ni-64
Zr-90
Zr-91
Zr-92
Zr-93
Moderating quality
Energy (eV)


Zr-94
Zr-95
Zr-96
Sn-116
Sn-120
Xe-131
Xe-135
Au-197
Moderating quality
Energy (eV)


Pb-0
Moderating quality
10^5
10^0
10^{-10}
10^0
10^{10}
Energy (eV)
Bi-209
Moderating quality
10^5
10^0
10^{-10}
10^0
10^{10}
Energy (eV)

B. MCNP Code

```
Optimized filter specification gradient ascent method
c Cell cards
1  0          1 -2 6 -7 8 -9 imp:n=1
2  1  -2.91   2 -3 6 -7 8 -9 imp:n=1
3  2  -2.340  3 -4 6 -7 8 -9 imp:n=1
4  0          4 -5 6 -7 8 -9 imp:n=1
5  0          -1:4:-5:6:-7:8 imp:n=0

c Defining the surfaces to make the structure of the filter/ moderator
c arrangement
1   PX -5
2   PX 0
3   PX 20
4   PX 21
5   PX 100
6*  PY 0
7*  PY 100
8*  PZ 0
9*  PZ 100

c Data cards, including source, tally, energy bin, material and problem
c cutoff definitions
SDEF ERG=2 PAR=1 NRM=1 DIR=1 X=-5 Y=D1 Z=D2 VEC=1
SI1  0. 100.
SI2  0. 100.
SP1  0. 1.
SP2  0. 1.
F1:N 5
E1 0.0001 8I 0.001 38I 0.040 5I 0.1 18I 2
F11:N 5
E11 0.001 0.020 2
M1 13027 0.25 9019 0.75
M2 5010 1
NPS 1000000
PRDMP 1000000 1000000 -1 5 0
```

C. Perl script

C1. Perl script in blocks

1

```
#!/bin/perl

#Optimalisatie door gebruik te maken van de "gradient ascent method"

@DF = ( );
@D1 = ( );
@D2 = ( );
@Ther = ( );
@Epi = ( );
@Fast = ( );
@Errther = ( );
@Errepi = ( );
@Errfast = ( );
@Errdf = ( );
@Precision = ( );
@DeltaD1 = ( );
@DeltaD2 = ( );
@gamma = ( );
$n = 0;
$d1 = 15;
$d2 = $d1+15;
$d4 = 200;
```

2

```
$precision = 100;

while ($precision > 0.1) {

   $n=$n+1;

   $d3 = $d2+1.5;

   open FILE, "+>GRAS$n.i";

   print FILE "Optimized filter specification gradient ascent method
   1  0          1 -2 7 -8 9 -10 imp:n=1
   2  1  -2.2    2 -3 7 -8 9 -10 imp:n=1
   3  2  -2.62   3 -4 7 -8 9 -10 imp:n=1
   4  3  -0.53   4 -5 7 -8 9 -10 imp:n=1
   5  0          5 -6 7 -8 9 -10 imp:n=1
   6  0          -1:6:-7:8:-9:10  imp:n=0

   1   PX -5
   2   PX 0
   3   PX $d1
   4   PX $d2
   5   PX $d3
   6   PX $d4
   7*  PY 0
   8*  PY 100
   9*  PZ 0
   10* PZ 100

   SDEF ERG=2 PAR=1 NRM=1 DIR=1 X=-5 Y=D1 Z=D2 VEC=1
   SI1  0. 100.
   SI2  0. 100.
   SP1  0. 1.
   SP2  0. 1.
   F1:N 6
   E1 0.000005 0.020 2
   M1 14000 0.33 8016 0.67
   M2 6000 1
   M3 3006 1
   NPS 1000000
   PRDMP 1000000 1000000 -1 5 0 \n";

   close FILE;
```

3

```
   #Run MCNP input file and wait till command is executed
   unless (fork) {
      exec("mcnp5 inp=GRAS$n.i o=GRAS$n");
   }
   wait;
```

4a

```
READ1:
   if (-r "GRAS$n") {

      open FILE, "+<GRAS$n" or die $!;
      @lines = <FILE>;

      #Search for lines with right data and...
      $line = 0;
      for (@lines) {
         if (/surface  6/) {
            $line1 = $line+2;
            $line2 = $line1;
         }
         if (/total/) {
            if ($line2 == $line1) {$line2 = $line-1};
         }
         $line++;
      }

      #...put those lines from MCNP output file in array
      $line = 0;
      for (@lines[$line1..$line2]) {
         @number=(split);
         $current[$line] = $number[1];
         $error[$line] = $number[2];
         $line++;
      }
```

4b

```
   #Thermal neutron current
   $THER = @current[0];
   print "$THER \n";

   if ($THER == 0) {
      $ERRTHER = 0;
   } else {
      $ERRTHER = @error[0];
   }

   @Ther = (@Ther, $THER);
   @Errther = (@Errther, $ERRTHER);

   #Epithermal neutron current
   $EPI = @current[1];

   print "EPI = $EPI \n";
   if ($EPI < 0.01) {
      goto END;
   }

   if ($EPI == 0) {
      $ERREPI = 0;
   } else {
      $ERREPI = @error[1];
   }

   @Epi = (@Epi, $EPI);
   @Errepi = (@Errepi, $ERREPI);

   #Fast neutron current
   $FAST = @current[2];

   if ($FAST == 0) {
      $ERRFAST = 0;
   } else {
      $ERRFAST = @error[2];
   }

   @Fast = (@Fast, $FAST);
   @Errfast = (@Errfast, $ERRFAST);

   #GOALFUNCTION (DF)
   $DF = $EPI/($THER+$EPI+$FAST);
   @DF = (@DF, $DF);

   print "DF = $DF\n";

} else {
   goto READ1;
}
```

5

```
  for ($i=1; $i<4; $i++) {

      if ($i=1) {

         $dikte1 = $d1;
         $d10 = $d1;
         @D1 = (@D1,$dikte1);
         $dikte2 = $d2-$d1;
         $d20 = $dikte2;
         @D2 = (@D2,$dikte2);
         $d1 = 1.05*$d1;
         $d11 = $d1;
         $d2 = $d1+$dikte2;
         $d3 = $d2+1.5;
         $n = $n+1;

         open FILE, "+>GRAS$n.i";
         close FILE;

#Then read data as in block 4a and b

         if ($i=2) {

         $d2 = 1.05*$d20;
         $d21 = $d2;
         $d1 = $d10;
         $d2 = $d1+$d2;
         $d3 = $d2+1.5;
         $n = $n+1;

         open FILE, "+>GRAS$n.i";
         close FILE;
```

6

```
if ($i=3) {

          $gamma = 1/(@DF[(1/3)*$n-1]); #This can be taken variable
          #$gamma = 50;
        @gamma  = (@gamma, $gamma);

        $DeltaD1 = $gamma*(($DFd1-@DF[(1/3)*$n-1])/($d11-$d10));
        $DeltaD2 = $gamma*(($DFd2-@DF[(1/3)*$n-1])/($d21-$d20));
        $precision = abs($DeltaD1)+abs($DeltaD2);

        $d1 = $d10+$DeltaD1;
        if ($d1 < 0) {$d1 = 0.01;}

        $d2 = $d20+$DeltaD2;
          if ($d2 < 0) {$d2 = 0.01;}

        if ($precision < 0.01) {
           @D1 = (@D1, $d1);
           @D2 = (@D2, $d2);
        }

        $d2 = $d1+$d2;


        print "De nieuwe Dikte 1 is $d1 en de nieuwe Dikte 2 is $d2.
DeltaDF1 = $DeltaD1. DeltaDF2 = $DeltaD2. \n";

      }

   }
```

7

```
@Precision = (@Precision, $precision);
   @DeltaD1 = (@DeltaD1, $DeltaD1);
   @DeltaD2 = (@DeltaD2, $DeltaD2);

   open DATA, "+>GRASMETHDATA";
   print DATA "Dikte1: @D1
   Dikte2: @D2
   Doelfunctie: @DF
   Thermisch: @Ther
   Epi: @Epi
   Fast: @Fast
   Errther: @Errther
   Errepi: @Errepi
   Errfast: @Errfast
   Errdf: @Errdf
   Precision: @Precision
   Gamma: @gamma
   DeltaD1: @DeltaD1
   DeltaD2: @DeltaD2 \n";

   close DATA;

}
```

8

```
 END:
print "Run is finished, you can have coffee now! \n";
```

C2. Perl script

```
#!/bin/perl

#Optimalisatie door gebruik te maken van de "gradient ascent method"

@DF = ( );
@D1 = ( );
@D2 = ( );
@Ther = ( );
@Epi = ( );
@Fast = ( );
@Errther = ( );
@Errepi = ( );
@Errfast = ( );
@Errdf = ( );
@Precision = ( );
@DeltaD1 = ( );
@DeltaD2 = ( );
@gamma = ( );
$n = 0;
$d1 = 15;
$d2 = $d1+15;
$d4 = 200;

$precision = 100;

while ($precision > 0.1) {

   $n=$n+1;

   $d3 = $d2+1.5;

   open FILE, "+>GRAS$n.i";

   print FILE "Optimized filter specification gradient ascent method
   1  0          1 -2 7 -8 9 -10 imp:n=1
   2  1  -2.2    2 -3 7 -8 9 -10 imp:n=1
   3  2  -2.62   3 -4 7 -8 9 -10 imp:n=1
   4  3  -0.53   4 -5 7 -8 9 -10 imp:n=1
   5  0          5 -6 7 -8 9 -10 imp:n=1
   6  0          -1:6:-7:8:-9:10  imp:n=0

   1   PX -5
   2   PX 0
   3   PX $d1
   4   PX $d2
   5   PX $d3
   6   PX $d4
   7*  PY 0
   8*  PY 100
   9*  PZ 0
   10* PZ 100

   SDEF ERG=2 PAR=1 NRM=1 DIR=1 X=-5 Y=D1 Z=D2 VEC=1
   SI1  0. 100.
   SI2  0. 100.
   SP1  0. 1.
   SP2  0. 1.
   F1:N 6
   E1 0.000005 0.020 2
```

```
M1 14000 0.33 8016 0.67
M2 6000 1
M3 3006 1
NPS 1000000
PRDMP 1000000 1000000 -1 5 0 \n";

close FILE;

unless (fork) {
   exec("mcnp5 inp=GRAS$n.i o=GRAS$n");
}
wait;

READ1:
if (-r "GRAS$n") {

   open FILE, "+<GRAS$n" or die $!;
   @lines = <FILE>;

   #Search for lines with right data and...
   $line = 0;
   for (@lines) {
      if (/surface  6/) {
         $line1 = $line+2;
         $line2 = $line1;
      }
      if (/total/) {
         if ($line2 == $line1) {$line2 = $line-1};
      }
      $line++;
   }

   #...put those lines from MCNP output file in array
   $line = 0;
   for (@lines[$line1..$line2]) {
      @number=(split);
      $current[$line] = $number[1];
      $error[$line] = $number[2];
      $line++;
   }

   #Thermal neutron current
   $THER = @current[0];
   print "$THER \n";

   if ($THER == 0) {
      $ERRTHER = 0;
   } else {
      $ERRTHER = @error[0];
   }

   @Ther = (@Ther, $THER);
   @Errther = (@Errther, $ERRTHER);

   #Epithermal neutron current
   $EPI = @current[1];

   print "EPI = $EPI \n";
   if ($EPI < 0.01) {
      goto END;
   }
```

```
   if ($EPI == 0) {
      $ERREPI = 0;
   } else {
      $ERREPI = @error[1];
   }

   @Epi = (@Epi, $EPI);
   @Errepi = (@Errepi, $ERREPI);

   #Fast neutron current
   $FAST = @current[2];

   if ($FAST == 0) {
      $ERRFAST = 0;
   } else {
      $ERRFAST = @error[2];
   }

   @Fast = (@Fast, $FAST);
   @Errfast = (@Errfast, $ERRFAST);

   #GOALFUNCTION (DF)
   $DF = $EPI/($THER+$EPI+$FAST);
   @DF = (@DF, $DF);

   print "DF = $DF\n";

} else {
   goto READ1;
}

for ($i=1; $i<4; $i++) {

   if ($i=1) {

      $dikte1 = $d1;
      $d10 = $d1;
      @D1 = (@D1,$dikte1);
      $dikte2 = $d2-$d1;
    $d20 = $dikte2;
      @D2 = (@D2,$dikte2);
      $d1 = 1.05*$d1;
    $d11 = $d1;
      $d2 = $d1+$dikte2;
      $d3 = $d2+1.5;
    $n = $n+1;

open FILE, "+>GRAS$n.i";

print FILE "Optimized filter specification gradient ascent method
1  0          1 -2 7 -8 9 -10 imp:n=1
2  1  -2.2    2 -3 7 -8 9 -10 imp:n=1
3  2  -2.62   3 -4 7 -8 9 -10 imp:n=1
4  3  -0.53   4 -5 7 -8 9 -10 imp:n=1
5  0          5 -6 7 -8 9 -10 imp:n=1
6  0          -1:6:-7:8:-9:10  imp:n=0

1   PX -5
2   PX 0
3   PX $d1
```

```
4   PX $d2
5   PX $d3
6   PX $d4
7*  PY 0
8*  PY 100
9*  PZ 0
10* PZ 100

SDEF ERG=2 PAR=1 NRM=1 DIR=1 X=-5 Y=D1 Z=D2 VEC=1
SI1  0. 100.
SI2  0. 100.
SP1  0. 1.
SP2  0. 1.
F1:N 6
E1 0.000005 0.020 2
M1 14000 0.33 8016 0.67
M2 6000 1
M3 3006 1
NPS 1000000
PRDMP 1000000 1000000 -1 5 0 \n";
close FILE;

      unless (fork) {
         exec("mcnp5 inp=GRAS$n.i o=GRAS$n");
      }
      wait;

      READ2:
      if (-r "GRAS$n") {

         open FILE, "+<GRAS$n" or die $!;
         @lines = <FILE>;

         #Search for lines with right data and...
         $line = 0;
         for (@lines) {
            if (/surface  6/) {
            $line1 = $line+2;
            $line2 = $line1;
            }
            if (/total/) {
               if ($line2 == $line1) {$line2 = $line-1};
            }
            $line++;
      }

      #...put those lines from MCNP output file in array
      $line = 0;
      for (@lines[$line1..$line2]) {
         @number=(split);
         $current[$line] = $number[1];
         $error[$line] = $number[2];
         $line++;
      }

      #Thermal neutron current
      $THER = @current[0];

      if ($THER == 0) {
         $ERRTHER = 0;
      } else {
```

```
         $ERRTHER = @error[0];
      }

      #Epithermal neutron current
      $EPI = @current[1];

      if ($EPI == 0) {
         $ERREPI = 0;
      } else {
         $ERREPI = @error[1];
      }

      #Fast neutron current
      $FAST = @current[2];

      if ($FAST == 0) {
         $ERRFAST = 0;
      } else {
         $ERRFAST = @error[2];
      }

      #GOALFUNCTION (DF)
      $DFd1 = $EPI/($THER+$EPI+$FAST);

      } else {
         goto READ2;
      }

   }

   if ($i=2) {

      $d2 = 1.05*$d20;
      $d21 = $d2;
    $d1 = $d10;
      $d2 = $d1+$d2;
      $d3 = $d2+1.5;
      $n = $n+1;

open FILE, "+>GRAS$n.i";

print FILE "Optimized filter specification gradient ascent method
1  0          1 -2 7 -8 9 -10 imp:n=1
2  1  -2.2    2 -3 7 -8 9 -10 imp:n=1
3  2  -2.62   3 -4 7 -8 9 -10 imp:n=1
4  3  -0.53   4 -5 7 -8 9 -10 imp:n=1
5  0          5 -6 7 -8 9 -10 imp:n=1
6  0          -1:6:-7:8:-9:10  imp:n=0

1   PX -5
2   PX 0
3   PX $d1
4   PX $d2
5   PX $d3
6   PX $d4
7*  PY 0
8*  PY 100
9*  PZ 0
10* PZ 100

SDEF ERG=2 PAR=1 NRM=1 DIR=1 X=-5 Y=D1 Z=D2 VEC=1
```

```
SI1  0. 100.
SI2  0. 100.
SP1  0. 1.
SP2  0. 1.
F1:N 5
E1 0.000005 0.020 2
M1 14000 0.33 8016 0.67
M2 6000 1
M3 3006 1
NPS 1000000
PRDMP 1000000 1000000 -1 5 0 \n";
close FILE;

      unless (fork) {
         exec("mcnp5 inp=GRAS$n.i o=GRAS$n");
      }
      wait;

      READ3:
      if (-r "GRAS$n") {

         open FILE, "+<GRAS$n" or die $!;
         @lines = <FILE>;

         #Search for lines with right data and...
         $line = 0;
         for (@lines) {
            if (/surface  6/) {
            $line1 = $line+2;
            $line2 = $line1;
         }
         if (/total/) {
            if ($line2 == $line1) {$line2 = $line-1};
         }
         $line++;
      }

      #...put those lines from MCNP output file in array
      $line = 0;
      for (@lines[$line1..$line2]) {
         @number=(split);
         $current[$line] = $number[1];
         $error[$line] = $number[2];
         $line++;
      }

      #Thermal neutron current
      $THER = @current[0];

      if ($THER == 0) {
         $ERRTHER = 0;
      } else {
         $ERRTHER = @error[0];
      }

      #Epithermal neutron current
      $EPI = @current[1];

      if ($EPI == 0) {
         $ERREPI = 0;
      } else {
```

```
            $ERREPI = @error[1];
         }

         #Fast neutron current
         $FAST = @current[2];

         if ($FAST == 0) {
            $ERRFAST = 0;
         } else {
            $ERRFAST = @error[2];
         }

         #GOALFUNCTION (DF)
         $DFd2 = $EPI/($THER+$EPI+$FAST);

         } else {
            goto READ3;
         }

      }

      if ($i=3) {

         $gamma = 1/(@DF[(1/3)*$n-1]); #This can be taken variable
         #$gamma = 50;
       @gamma  = (@gamma, $gamma);

       $DeltaD1 = $gamma*(($DFd1-@DF[(1/3)*$n-1])/($d11-$d10));
       $DeltaD2 = $gamma*(($DFd2-@DF[(1/3)*$n-1])/($d21-$d20));
       $precision = abs($DeltaD1)+abs($DeltaD2);

       $d1 = $d10+$DeltaD1;
       if ($d1 < 0) {$d1 = 0.01;}

       $d2 = $d20+$DeltaD2;
         if ($d2 < 0) {$d2 = 0.01;}

       if ($precision < 0.01) {
          @D1 = (@D1, $d1);
          @D2 = (@D2, $d2);
       }

       $d2 = $d1+$d2;


       print "De nieuwe Dikte 1 is $d1 en de nieuwe Dikte 2 is $d2.
DeltaDF1 = $DeltaD1. DeltaDF2 = $DeltaD2. \n";

      }

   }

   @Precision = (@Precision, $precision);
   @DeltaD1 = (@DeltaD1, $DeltaD1);
   @DeltaD2 = (@DeltaD2, $DeltaD2);

   open DATA, "+>GRASMETHDATA";
   print DATA "Dikte1: @D1
   Dikte2: @D2
   Doelfunctie: @DF
   Thermisch: @Ther
```

```
   Epi: @Epi
   Fast: @Fast
   Errther: @Errther
   Errepi: @Errepi
   Errfast: @Errfast
   Errdf: @Errdf
   Precision: @Precision
   Gamma: @gamma
   DeltaD1: @DeltaD1
   DeltaD2: @DeltaD2 \n";

   close DATA;

}

END:
print "Run is finished, you can have coffee now! \n";
```