The Thorium fuel cycle in nuclear reactors

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Thesis presented to obtain the degree of Physicist

Bogotá, Colombia

October 20, 2024

Regards

Resumen

Palabras clave:

Abstract

Keywords:

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1. Introduction

Nuclear reactors remain a highly debated topic in both scientific and political circles. While they play a crucial role in generating clean energy, significant challenges related to safety, environmental impact, and economics persist. For instance, the time and capital required to deploy a nuclear reactor are substantial [1]. This thesis aims to examine the current state of nuclear reactors, focusing on their design, operations, and the potential of thorium fuel cycles. It will explore the benefits and drawbacks of various nuclear fuel cycles and reactor designs, as well as their future prospects.

Nuclear energy is often associated with atomic weapons due to the events of World War II and the subsequent arms race during the Cold War [2].However, following the end of the Cold War, the focus of the nuclear industry shifted towards civilian applications, particularly energy production, largely driven by growing concerns over greenhouse gas emissions. One of the key advantages of nuclear energy is that it produces power without emitting greenhouse gases [2].

The development of nuclear reactors began in the mid-20th century, initially driven by military needs, particularly for the propulsion of naval vessels, such as submarines and aircraft carriers. Nuclear power offered significant advantages, especially in submarines, where the lack of a need for combustion allowed them to operate underwater for extended periods. In the case of aircraft carriers, nuclear propulsion freed up space previously used for fuel oil, allowing more room for aviation fuel and other supplies [2].

Several countries explored the use of nuclear reactors for civilian ship propulsion. The U.S. nuclear-powered merchant ship, 'Savannah', operated briefly during the 1960s and 1970s, demonstrating the technical feasibility of nuclear propulsion for commercial vessels, though it proved economically unviable. Other nations, including Japan, Germany, and the Soviet Union, also experimented with nuclear-powered merchant ships. Notably, Germany's ore carrier, 'Otto Hahn', operated successfully for a decade before being decommissioned due to high costs. In contrast, the Soviet Union's icebreaker 'Lenin' demonstrated the value of nuclear power in extreme environments, leading to the construction of additional nuclear-powered icebreakers [2].

Nuclear power was also explored for other applications. In 1945, Eugene Wigner and Alvin Weinberg proposed a liquid fuel reactor design [3]. The Oak Ridge National Laboratory (ORNL) investigated a potential nuclear application of this concept to jet engines [3]. From 1949 to 1961, the U.S. invested approximately one billion dollars in the Aircraft Nuclear Propulsion Project (ANP). This project aimed to develop a nuclear-powered aircraft capable of long-range missions, a crucial priority during the early Cold War. However, with the advent of long-range ballistic missiles, the need for such an aircraft diminished, and the project was ultimately terminated [2].

At the time, there were concerns that the global supply of ^{235}U would be insufficient to meet future energy demands. Weinberg and his colleagues recognized that molten salt reactors (MSRs) could be used to breed ^{233}U from thorium [3]. Between 1965 and 1969, ORNL successfully operated an MSR experiment for 15 months, achieving an impressive 87% operational uptime, even utilizing ^{233}U as fuel [3]. Despite this success, the MSR program was eventually discontinued as other nuclear concepts received greater political support [3].

This thesis aims to explore the potential of the thorium fuel cycle in the nuclear industry and its prospects for the near future. The research investigates the benefits and challenges associated with thorium fuel, as well as the various proposed implementations for integrating this cycle into commercial reactors.

2. The Physics Behind Nuclear Reactors

The level of interactions within a nuclear reactor is governed by neutron transport [4]. In this chapter we will delve into the physical details that drive a nuclear reactor.
The theory of relativity tells us that there is a direct relation between mass and energy, expressed by the equation $E = mc^2$. Nuclear reactors are the most well-known practical application of this theory, as they harness some of the energy held in the nucleus's mass to generate electricity for our society [5]. To understand the wide difference between chemical reactions, used in fossil fuel generations methods, and nuclear energy, we will study and compare the amount of energy each one generates.
The combustion of coal is given by the chemical reaction $C + O_2 \rightarrow CO_2$ while the nuclear energy production uses the reaction: neutron+$^{235}U \rightarrow$ Fission's products. Each carbon atom combusted produces approximately 4.0 eV, whereas each uranium atom fissioned produces around 200 million eV (200 MeV) [5]. There are eight orders of magnitude in energy release.

2.1. Binding energy

If one adds the mass of all the nucleons in a nucleus, and then compared it with the mass of the nucleus, you would know that these two values do not match. This discrepancy is known as the mass defect [4].

$$\Delta = [Zm_p + (A - Z)m_n] - m(A, Z) \tag{2-1}$$

Disassembling the nucleus into nucleons will results in an increase in mass equivalent to the mass defect. This energy is known as the binding energy of the nucleus $BE = \Delta c^2$, where

Δ is the mass defect. This energy can be normalized by dividing it by the total amount of nucleons, resulting in the binding energy per nucleon, as follows [5]:

$$\Delta c^2/(Z+N) = \Delta c^2/A \tag{2-2}$$

Fig (**2-1**) shows the binding energy per nucleon for various isotopes, highlighting the stability of different nuclei. The peak of the curve, around iron (Fe), highlights the most stable nuclei, with the highest binding energy per nucleon.

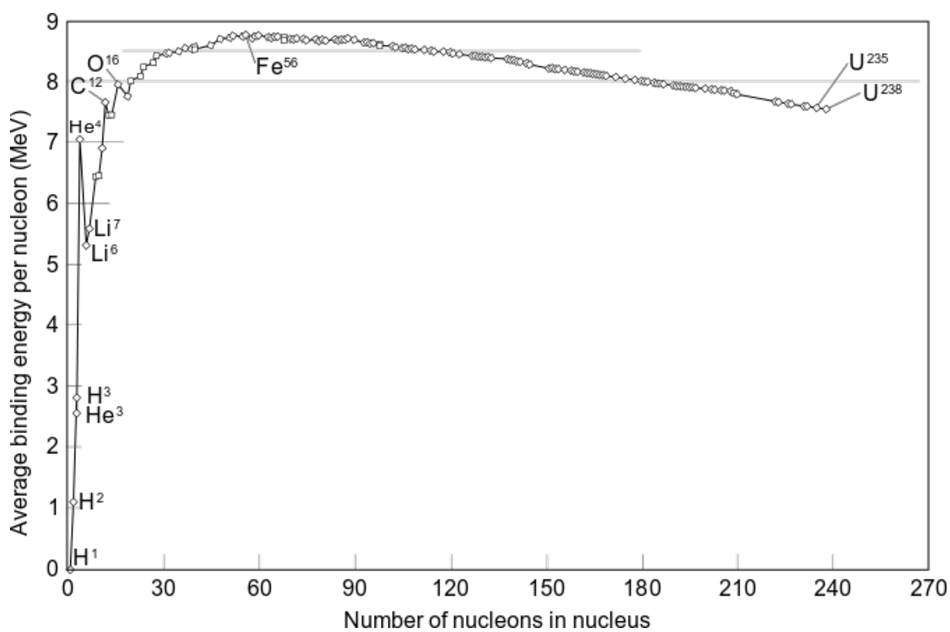

Figure 2-1.: This figure shows the binding energy per nucleon as a function of the number of nucleons. Source : [6]

Processes that result in nuclei with more binding energy per nucleon convert mass into energy [4]. There are two possible processes in which this may happen: fission and fusion reactions. Fusion reactions happen when two light nuclei combine and form a heavier nucleus [5]. On the contrary, fission occurs when a heavier nucleus splits to form lighter nuclei [4]. Fission is the process on which nuclear reactors are based.

2.1.1. Liquid-Drop Model

The liquid-drop model, one of the first nuclear models, was proposed by Bohr in 1935. It is based on the short range of nuclear forces as well as the additivity of volumes and binding energies. The basic idea is that nucleons interact strongly with their neighbours, similar to how molecules interact in a drop of water [7].

Based on this model, in 1935 Bethe and Weizsäcker made an excellent parametrization of the binding energies of nuclei in their ground state. This formula extends the idea of the liquid-drop model to incorporate two new ingredients, related to quantum properties of the nuclear mater. The first one is the asymmetric energy which tends to stabilize nuclei with equal number of protons and neutrons. The other is the pairing energy which favors paired fermions [7]. The formula is composed by five therms:

- The first parameter in the formula is related to the volume ($a_v = 15.753MeV$). This term reflects the nearest neighbor interactions and leads to a constant binding energy per nucleon.
- The term a_s lowers the binding energy and is related to the surface of the nucleus. While internal nucleus feel isotropic interactions, nucleus on the surface feel forces coming only from the inside. Since superficial area of a sphere is $4\pi R^2$ and $R \sim A^{2/3}$, this therm is proportional to $A^{2/3}$.
- a_c is related to the Coulomb repulsion of protons therefore lowers binding energy of the nucleus. Coulomb potential is proportional to Q^2/R thus $a_c \sim Z^2/A^{1/3}$.
- While a_c favors neutron excess over protons, the term a_a favors symmetry between protons and neutrons related to the isospin.
- Finally, $\delta(A)$ is a quantum pairing term.

The Bethe-Weizsäcker's formula is:[7]

$$B(A,Z) = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(N-Z)^2}{A} + \delta(A) \tag{2-3}$$

Since this is a empirical formula each parameter a_i has to be fitted to the data. This fitting process results in the following values:

- $a_v = 15.753 MeV$
- $a_s = 17.804 MeV$
- $a_c = 0.7103 MeV$
- $a_a = 23.69 MeV$
- $\delta(A) = \begin{cases} 33.6A^{-3/4} & \text{if } N \text{ and } Z \text{ are even} \\ -33.6A^{-3/4} & \text{if } N \text{ and } Z \text{ are odd} \\ 0 & \text{if } A = N + Z \text{ is odd} \end{cases}$

2.1.2. Instability of Isotopes

Induced fission occurs when a probe transfers energy into a nucleus, leaving it in an excited state, which may then split into two fragments of similar size. There are various kinds of probe, but for induced fission reactions, neutrons are the most effective because they do not have an electric charge. Therefore, they do not experience Coulomb repulsion, allowing them to penetrate deeper into the nucleus, bringing energy and causing a rearrangement in the shell structure of the nucleus.[8]

For instance suppose and spherical nucleus with:

$$V = \frac{4}{3}\pi R^3$$
$$S = 4\pi R^2$$

We will explore the effects of a small deformation like an prolate spheroid. Since nuclear mater is incompressible, the volume will not change, at least to first order. Consider a small deformation, $\epsilon << 1$:

$$a = R(1+\epsilon); b = R(1+\epsilon)^{-1/2}$$
$$V = \frac{4}{3}\pi ab^2 = \frac{4}{3}\pi R^3$$

With these definitions, the volume remains constant, but the surface area increases. Using a Taylor series expansion for small ϵ, we have:

$$\frac{a}{b} = 1 + \frac{3}{2}\epsilon + \frac{3}{8}\epsilon^2 + \cdots$$

Also,

$$\left(\frac{b}{a}\right)^2 = 1 - 3\epsilon + 6\epsilon^2 - 10\epsilon^3 + \cdots$$

Given $\frac{\arcsin\epsilon}{\epsilon} = 1 + \frac{1}{2}\epsilon - \frac{13}{40}\epsilon^2 + \cdots$, we get:

$$\left(\frac{b}{a}\right)^2 \left(\frac{\arcsin\epsilon}{\epsilon}\right) = 2\left(1 + \epsilon + \frac{2}{3}\epsilon^2 + \cdots\right)$$

Substituting into the surface area S:

$$S = 4\pi R^2 \left(1 + \frac{2}{5}\epsilon + \cdots\right) \tag{2-4}$$

Finally, considering the average distance between nucleons inside the deformed nucleus:

$$\bar{R} = R\left(1 + \frac{1}{5}\epsilon^2 + \cdots\right)$$
$$\bar{R}^{-1} = R^{-1}\left(1 - \frac{1}{5}\epsilon^2 + \cdots\right) \tag{2-5}$$

Knowing how $\bar{R}$ and S change in the nucleus with the small deformation **Eq.**(2-5) and **Eq.**(2-4) respectively, we can evaluate the binding energy **Eq.**(2-3) and see how it changes. The

Coulomb and the surface terms are the ones that change. The following analysis will detail these changes:

$$\Delta E = B(\epsilon) - B(0)$$
$$\Delta E = \left(-\frac{2}{5}a_s A^{2/3} + \frac{1}{5}a_c z(z-1)A^{-1/3}\right)\epsilon^2$$

If $\Delta E > 0$, then $B(\epsilon) > Bb(\epsilon = 0)$. This means that the deformed nucleus is lighter that the spherical one, resulting in an tendency towards stretching in the nucleus, which leads to fission [9]. We will focus on the conditions that lead to $\Delta E > 0$:

$$-\frac{2}{5}a_s A^{2/3} + \frac{1}{5}a_c z(z-1)A^{-1/3} > 0$$
$$\frac{1}{5}a_c z(z-1)A^{-1/3} > \frac{2}{5}a_s A^{2/3}$$
$$(z \gtrsim 90) \rightarrow z(z-1) \approx z^2$$
$$a_c Z^2 > 2a_s A$$
$$Z^2/A > \frac{2a_s}{a_c}$$

The right side of the expression can be approximated $\frac{2a_s}{a_c} \approx 47$ which leave us we the condition [9]:

$$\frac{Z^2}{A} > 47. \tag{2-6}$$

A nucleus with this property is completely unstable to fission. When discussing about nuclear reactors, we want isotopes that are prone to fission, but this probability should not be too high because spontaneous fission would dominate the reaction, reducing the efficiency of the reactor [8]. Nuclei with $Z > 90$ and $A > 230$ undergo fission relatively easily, either through induced or spontaneous processes.[5]

2.1.3. Valley of Instability

The presence of Coulomb and asymmetric terms in the binding energy **Eq.**(2-3) implies the existence of a maximum in the binding energy for a given A, as a function of Z [7]. To find this relation, we set $\partial B/\partial Z = 0$, as shown in the following expression:

$$\left.\frac{\partial B}{\partial Z}\right|_{A=\text{const}} = -2a_c\frac{Z_{\min}}{A^{1/3}} + 2a_a\frac{(N - Z_{\min})}{A}$$

Setting this expression to zero and replacing $N = A - Z$, we get:

$$\begin{aligned} 0 &= -2a_c\frac{Z_{\min}}{A^{1/3}} + 2a_a\frac{(A - 2Z_{\min})}{A} \\ 0 &= -a_c\frac{Z_{\min}}{A^{1/3}} + a_a - 2\frac{Z_{\min}}{A} \\ Z_{\min} &= \frac{A}{2 + a_c A^{2/3}/(2a_a)} \end{aligned}$$

This expression can be approximated by $N = Z = A/2$ and $a_c/a_a \approx 0.0075$ [7]. This leaves us with the expression:

$$Z_{\min} \approx \frac{A}{2}\,\frac{1}{1 + 0.0075\,A^{2/3}} \tag{2-7}$$

The **Eq.**(2-7) tells us which is the most stable isotope for a given A. This information will be helpful later in the document when we discuss the requirement of stable isotopes for the reactor fuel.

2.2. Nuclear Fission

A first approximation to study the probability of a nuclear fission, one can suppose that the fission fragments live within the nucleus and fission takes place when one of them surpasses the Coulomb barrier [8].

For instance, consider the fission reaction of a nucleus, specifically ^{235}U undergoing an induced fission reaction. We will delve into this type of fission later in the document. This

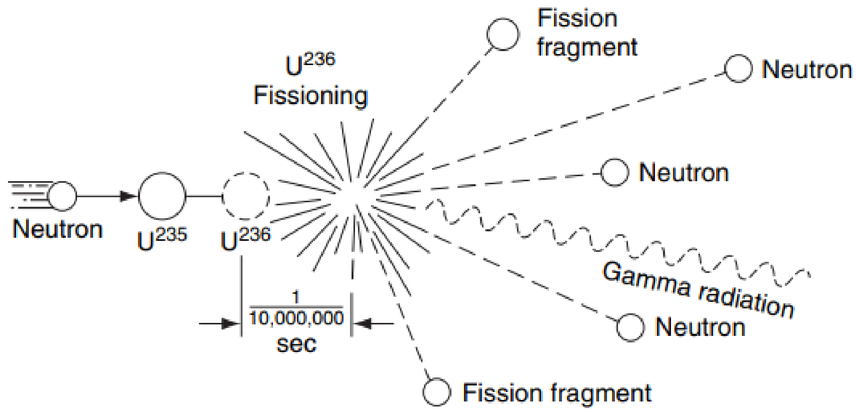

Figure 2-2.: Detailed Schematic of a Nuclear Fission Reaction. Source: [4].

reaction results in many products such as neutrons, fission fragments and radiation, as shown in **Fig** (**2-2**). Each of these products plays its role in a nuclear reactor.

Subsequently, suppose that the nucleus splits in two similar fragments, ${}^{119}_{46}Pd$. To compute the energy liberated in the reaction we just need to compute the difference in binding energy between ${}^{238}U$ and $2 \times {}^{119}Pd$, which is equal to 214 MeV.

To continue, we compute the Coulomb barrier, knowing that $R = R_1 + R_2$, $R_2 = R_1$ and $R_1 = R_0(119)^{1/3} = 6\,\mathrm{fm}$:

$$V = \frac{1}{4\pi\epsilon_0}\frac{Z_1 Z_2 e^2}{R}$$

$$R = 12\,\mathrm{fm}$$

$$Z_1 = Z_2 = 46$$

$$V = 253\,\mathrm{MeV}$$

The excitation energy of the fragments inside ${}^{238}U$ is 214 MeV and the height of the Coulomb barrier is 253 MeV. This values are not that different, which makes the probability non-zero for one of the fragments escaping the nucleus because of quantum tunneling. This calculation is a mere sketch of what a real calculation needs to consider. For example, if we choose the two fragments to be ${}^{79}_{30}Zn$ and ${}^{159}_{62}Sm$ the Coulomb barrier will be reduced to 221. In more sophisticated version of these calculations, two new parameters will be added:

- Fission barrier

- activation energy

These more sophisticated calculation are based on the liquid-drop model and give us an idea of the activation energy, the energy required for a nucleus to surpass the fission barrier and fission [9].
When a neutron is absorbed into a heavy nucleus resulting in a compound nucleus, the binding energy per nucleon decreases. For some nuclei, such as ${}^{233}_{92}U$, ${}^{235}_{92}U$, ${}^{239}_{92}Pu$, this decrease is so significant that the compound nucleus will undergo fission with high probability, even if the neutron has very low energy [4]. A compound nucleus is an excited nucleus which decays via multiple paths, depending on the isotope.

2.2.1. Fission Products

Fission is an asymmetric process, this means the two resulting fragments have different masses. However, the probability that the two fragments have the same mass is close to zero, which is not well understand [8].
Fission fragments are unstable because they neutron excess [5]. When a nucleus undergoes fission, it not only produces fragments but also emits neutrons, known as prompt neutrons. This emission changes the proton-to-neutron ratio of the fragments. Nonetheless, these fragments still lie about the stability curve in **Fig** (**2-3**). Some of these nuclei, less than 1%, decay by delayed-neutron emission, most of the fragments decay via beta emission or gamma rays. For example:

$$n + {}^{235}_{92}U \rightarrow {}^{140}_{54}Xe + {}^{94}_{38}Sr + 2n + 200MeV$$

${}^{140}_{54}Xe$ follows the chain of reactions:

$${}^{140}_{54}Xe \xrightarrow{\beta} {}^{140}_{55}Cs \xrightarrow{\beta} {}^{140}_{56}Ba \xrightarrow{\beta} {}^{140}_{57}La \xrightarrow{\beta} {}^{140}_{58}Ce$$

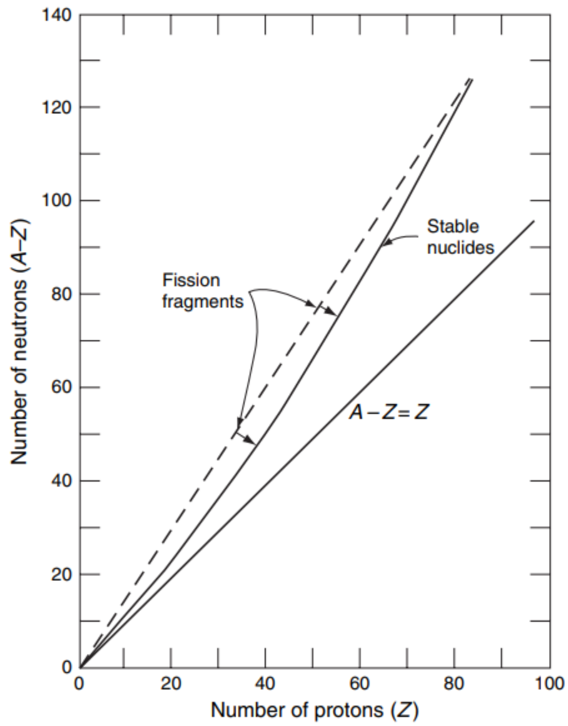

Figure 2-3.: Graph illustrating the relationship between the number of neutrons and the number of protons in nuclei. Source: [5]

This process shows only one of the 40 possible pairs that results from fission [5]. These fragments are highly radioactive and, in some cases, they can produced delayed neutron. Prompt and delayed neutrons play and fundamental role in the dynamics of a nuclear reactor.

2.2.2. Fission Cross Sections

Next we are going to focus on σ known as the nuclear reaction cross-section, which is a value that quantifies the probability of a nuclear reaction occurring [4]. This parameter is expressed in terms of the number of neutrons traveling with speed v a distance dx in a material with N nuclei per unit volume

$$\sigma := \frac{\text{reaction rate}}{nvNdx} \tag{2-8}$$

σ has units of area, consistent with the idea that σ is an effective area of interaction. That

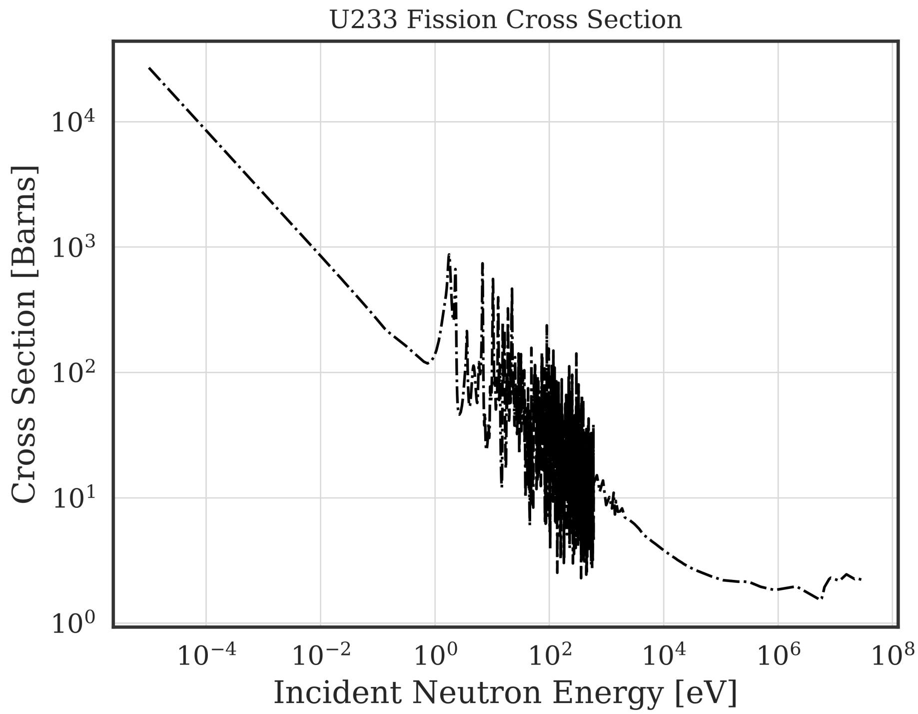

Figure 2-4.: Fission cross section of ^{233}U. Data retrieved from [10]

is why is called 'cross-section'. Typically, this parameter is measured in Barns. 1barn = $10^{-24}cm$ [4].

The fission cross section (σ_f), represents the probability that the interaction of a neutron and a nucleus will result in fission [4]. The probability peaks when the energy delivered to the nucleus, matches the energy difference between an excited state and the ground state of the compound nucleus. This phenomenon is known as resonances [4].

^{238}U fissions only by *fast neutrons* which are neutrons of high energy (energies around MeV). However, this cross section is small compared to others [8]. On the other hand, ^{235}U and ^{239}Pu undergo fission with neutrons across all energy spectra present in a nuclear reactor [8], as shown in **Fig** (**2-4**), including its resonances, which corresponds to the peaks in the graph.

2.3. Abundances of Isotopes

We already explored the instability of isotopes. Relation **Eq.**(2-6) give us an idea of how prone is a nucleus to fission. For instance, if we compute this parameter for the following nuclei, we get:

$$^{208}_{82}Pb \rightarrow 32.33$$
$$^{232}_{90}Th \rightarrow 34.91$$
$$^{238}_{92}U \rightarrow 35.56$$
$$^{235}_{92}U \rightarrow 36.02$$
$$^{233}_{92}U \rightarrow 36.33$$
$$^{239}_{94}Pu \rightarrow 36.97$$
$$^{252}_{94}Cf \rightarrow 38.11$$

All isotopes can undergo fission if they are hit with enough energy. In nuclear physics, probes usually have kinetic energies around MeV. Lead (Pb) is a very stable isotope. Isotopes, including Thorium-232 (^{232}Th) and Uranium-238 (^{238}U), have a non-zero probability of fission, yet their cross-sections are small. In contrast, isotopes, such as ^{235}U, ^{233}U and ^{239}Pu, are more prone to fission. Nuclei over Plutonium (Pu) can undergo spontaneous fission. This condition worsens for isotopes with $Z^2/A \geq 39$ which have infinitesimally small mean life [8]. Bringing this in mind, we can estimate some ranges for the stability of isotopes:

$$Z^2/A < 35 \rightarrow \text{Too stable}$$
$$Z^2/A \sim 35 \rightarrow \text{Fissile but not that much}$$
$$Z^2/A \sim 36 \rightarrow \text{Prone to fission}$$
$$Z^2/A \sim 38 \rightarrow \text{Spontaneous fission}$$
$$Z^2/A \gtrsim 39 \rightarrow \text{Too unstable}$$
$$Z^2/A > 47 \rightarrow \text{Not possible}$$

Besides, we have to look for isotopes that are close to the bottom of the valley of stability **Eq.** (2-7). Those far away from the valley will decay via $\beta^{+/-}$, α, neutron or proton evaporation [8]. This leaves us with three possible isotopes:

$$
\begin{aligned}
{}^{233}U &\rightarrow \tau = 160000\,\text{years} \\
{}^{235}U &\rightarrow \tau = 700\,\text{million years} \\
{}^{239}Pu &\rightarrow \tau = 24000\,\text{years}
\end{aligned}
$$

For an approximation of how much of each material is available on Earth, we are going to compare their mean life with the lifespan of Earth which is around 4.54 billion years. ${}^{239}Pu, \tau = 24000\,\text{years}$ This means it has passed 187000 mean lifespans since the creation of Earth, which indicates there is no plutonium left on earth. Something similar happens for ${}^{233}U$. Quite the contrary is the case of ${}^{235}U$ which has a mean life comparable to earth's age, which means there is ${}^{235}U$ on the planet but not that much.
The uranium available on Earth is known as 'natural uranium' (${}^{Nat}U$). Its composition is :

$$
\begin{cases}
{}^{238}U & \rightarrow 99.274\% \\
{}^{235}U & \rightarrow 0.720\% \\
{}^{234}U & \rightarrow 0.005\%
\end{cases}
$$

These isotopes are the ones that could be used as initial nuclear fuel for a nuclear reactor [8].

2.3.1. Notation

Latter on this document an special notation will be used to indicate the isotopes discussed here. The reader may notice the following pattern:

$$Th \to Z = 90$$
$$Pu \to Z = 94$$
$$Z \in [90, 94]$$

As well as :

$$^{232}Th \to A = 232$$
$$^{239}Pu \to A = 239$$
$$A \in [232, 239]$$

So we can think that we have the 'general case':

$$^{23b}_{9a}X \to \begin{cases} a = 0, 1, 2, 3, 4 \\ b = 2, 3, 4, 5, 6, 7, 8, 9 \end{cases}$$

So we can use this two numbers to refer to a certain isotope. For example:

$$^{232}_{90}Th \to 02$$
$$^{235}_{92}U \to 25$$
$$^{238}_{92}U \to 28$$

2.3.2. Fissionable and Fertile Material

Having introduced the fuel of a nuclear reactor, now we have to distinguish between two sub classes of fissionable material. Firstly, we have fissile nuclei which are the ones that undergo fission when they are irradiated by neutrons of some energy. For example ^{235}U is fissile. Secondly, we have fertile material which can undergo fission only by high energy neutrons. However, fertile materials can become fissile if they captures neutrons, transmutating via β decays or capturing neutrons again. This is the case of Thorium-232 (^{232}Th) and Uranium-238 (^{238}U).

$$n + {}^{238}_{92}U \rightarrow {}^{239}_{92}U^{*} \xrightarrow{\beta^-} {}^{239}_{93}Np \xrightarrow{\beta^-} {}^{239}_{94}Pu$$

$$n + {}^{232}_{90}Th \rightarrow {}^{233}_{90}Th^{*} \xrightarrow{\beta^-} {}^{233}_{91}Pa \xrightarrow{\beta^-} {}^{233}_{92}U$$

The crust of Earth has at least three times more Thorium-232 than Uranium [11]. Using this material to breed ^{233}U is the idea behind a Thorium fuel cycle. However, a breeding chain reaction is more difficult to sustain than a fission chain reaction [8].

2.4. Neutron Interactions

In order to produce energy, a nuclear reactor must sustain an equilibrium between the neutrons generated within the core and the neutrons lost[2].To achieve this, a nuclear reactor must sustain an induced fission chain reaction. In this process, neutrons, produced by fission, induced new fissions in other fissile nuclei [2]. These new fissions produce more neutrons, which induce further reactions, repeating the process. **Fig** (**2-5**) illustrates this process.
In each fission of ^{235}U, an average of 2.4 neutrons are produced [5]. We have already seen that around 200 MeV of energy is liberated after the fission of ^{235}U. Nonetheless, this energy is released as kinetic energy of the fission fragments (FF) and is eventually dissipated as heat.

2.4.1. Neutron Multiplication

The reaction represented in **Fig** (**2-5**) can be described in terms of a parameter known as 'multiplication factor', denoted as k [5]. The factor is defined as the number of neutrons produced in one generation divided by the number of neutrons produced in the preceding generation.

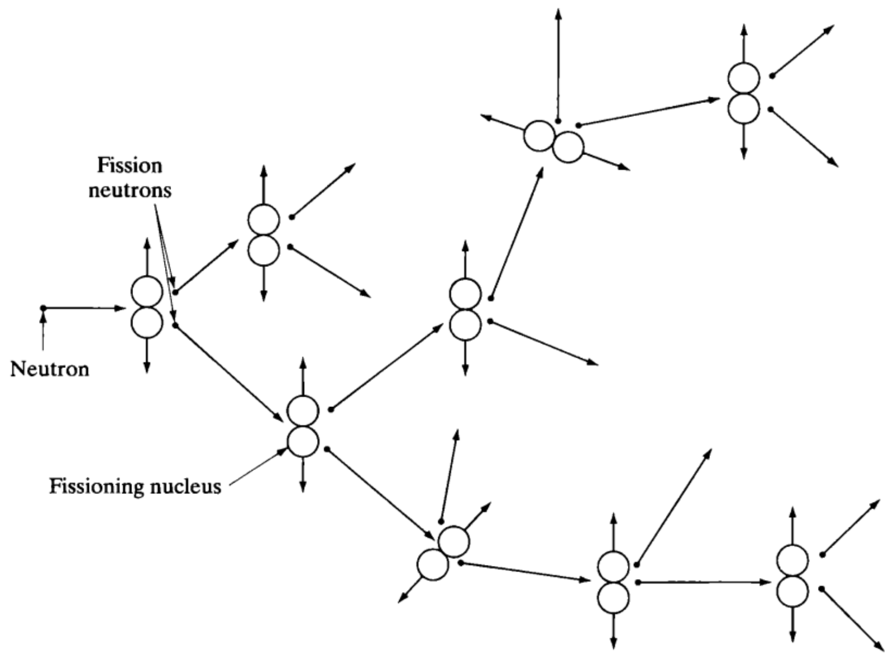

Figure 2-5.: Fission reaction chain schematic. Source: [5]

$$k := \frac{\text{Number of fission's neutrons produced in one generation}}{\text{Number of fission's neutrons produced in the preceding generation}} \tag{2-9}$$

In addition, if we want to estimate the number of neutrons produced in one generation, we need to use l, which is the lifespan of a neutron inside the reactor [5]. This is the time between the production and the absorption of neutrons. Suppose that there are n_0 neutrons at $t = 0$, then, we can use the following formula to compute the number of neutrons of the ith generation:

$$n(t) = n_0 k^{t/l} \tag{2-10}$$

There are three possibilities for the values of k:

$$k = \begin{cases} k > 1 : \text{“Supercritical”. Neutrons increases exponentially.} \\ k = 1 : \text{“critical”. The number of neutrons remains constant.} \\ k < 1 : \text{“Subcritical”. The number of neutrons decreases.} \end{cases}$$

2.4.2. Heat Produced by the Fuel

Around 8% of the 200 MeV of the energy produced by fission corresponds to the gamma rays associated with the beta decays of fission products [5]. Therefore, after a shutdown, a reactor that has been operating a for a time will keep radiating a significant amount of heat [5]. The heat produced after shutdown due to beta and gamma decays could be computed using the Wigner-Way formula.

$$P_d(t) = 0.0622 P_0[t^{-0.2} + (t_0 + t)^{-0.2}] \tag{2-11}$$

Where $P_d(t)$ is the power generated at time t, P_0 is the power of the reactor before the shutdown and t_0 is the time of power operation before the shutdown. Due to the decay heat produced after the shutdown, the reactor must be refrigerated to prevent overheating for a considerable period of time [5].

2.5. Microscopic and Macroscopic Cross Sections

After the previous discussion on nuclear fuel, we want to determine how neutrons interact with the material inside the reactor. To achieve this, let us consider a beam of neutrons traveling in the $+x$ direction. The intensity of the beam is given by $I = n'''v$, where n''' [1] is the volumetric neutron's density and v is the velocity at which all of the neutrons are traveling [5].

We assume that a neutron that collides with a nucleus is either absorbed or scattered into a different direction, reducing the number of neutrons traveling in the same direction [5]. This causes a decline in the intensity of the beam.

Let $I(x)$ be the intensity of the beam after penetrating a distant x in the material. Then, if the beam travels an additional infinitesimal distance dx, some neutrons will be removed. This removal is proportional to the number of nucleus in this region denoted as N and the cross-section, σ [5]. Therefore, we have:

[1] In this notation, quantities marked with triple primes ($'''$) represent volumetric densities, double primes ($''$) indicate surface densities, and single primes ($'$) denote linear densities.

$$I(x + dx) = (1 - N\sigma dx)I(x)$$

If $I(0) = I_0$ and applying the derivative:

$$\frac{d}{dx}I(x) = -N\sigma I(x)$$

Solving the differential equation an integrating from 0 to x:

$$I(x) = I_0 e^{-N\sigma x} \tag{2-12}$$

2.5.1. Macroscopic Cross Section

After this result, we want to introduce the macroscopic cross section, defined as:

$$\Sigma := N\sigma \tag{2-13}$$

Where σ refers to the microscopic cross section, measured in $cm^2/nucleus$, and N is still the volumetric nuclei density, measured in $nuclei/cm^3$. Then, the macroscopic cross section must have units of cm^-1.

Replacing $N\sigma$ in **Eq.**(2-12) with Σ, we obtain a macroscopic version of the flux. We can interpret this collided flux as a probabilistic distribution indicating the likelihood of a neutron reaching a depth x into a material without colliding [5].

$$I(x) = I_0 e^{-\Sigma x}$$

Dividing $I(x)$ by I_0, we obtain the fraction of neutrons that have reached a distance x without colliding. Interpreting $\frac{dI}{dx} = -\Sigma I(x)$ as the probability of a neutron having its first collision in the next dx, we have:

$$p(x)dx = (\Sigma dx)(\frac{I(x)}{I_0}) = \Sigma e^{-\Sigma x}dx$$

We can compute the mean free path λ, the mean distance traveled by a neutron between collisions, as [5]:

$$\lambda = \int_0^\infty xp(x)dx = \int_0^\infty x\Sigma e^{-\Sigma x}dx = \frac{1}{\Sigma}$$

2.6. Nuclei Density (N)

The Avogadro's number is the total of molecules in a mole of a substance, $N_0 = 0.6023 \cdot 10^24$ [5]. In order to compute the density of the molecule of a substance, we have to divide N_0 by the molecular wight A and, finally, multiply it by the density of the substance ρ [5]:

$$N = \rho N_0/A$$

Replacing this in **Eq.**(2-13) we have:

$$\Sigma = \frac{\rho N_0}{A}\sigma$$

Now if we apply this formula to an chemical element we have to consider that this element, in reality, exist in nature as a mixture of isotopes. To adjust the formula to this case we denote N^i/N as the atomic fraction of the isotope with A_i atomic weight, Thus we define the atomic weight of the mixture as [5]:

$$A = \sum_i (N^i/N)A_i,$$

where $N = \sum_i N^i$. Applying this to get the macroscopic cross section we get:

$$\Sigma = \frac{\rho N_0}{A} \sum_i \frac{N^i}{N} \sigma^i \tag{2-14}$$

Where σ^i is the microscopic cross section of the ith isotope.

In many cases material are combined using volume fractions. Once again, we want to make adjustment to our equation to consider this situation. Let V_i/V the volume fraction where $V = \sum_i V_i$, the cross section of the mixture is [5]:

$$\Sigma = \sum_i (V_i/V) N_i \sigma^i \tag{2-15}$$

.

To compute each of the nuclei number density we make use of the density of the ith nuclei ρ_i and its atomic weight A_i

$$N_i = \rho_i N_0 / A_i$$

The expression in **Eq.**(2-15) can be re written in terms of the macroscopic cross section of its components.

$$\Sigma = \sum_i (V_i/V) \Sigma^i$$

Where $\Sigma^i = N_i \sigma^i$. This expression can also be written in terms of mass fractions. Applying the same idea as before we get:

$$\sigma = \sum_i (M_i/M) \frac{\rho N_0}{A_i} \sigma^i$$

Where $M_i/M = \rho_i V_i / (\rho_i V)$ is the mass fraction, $M = \sum_i M_i$ and $\rho = M/V$.

2.6.1. Enriched Uranium

We have already mentioned that in nature uranium is found as a mixture of two main isotopes: 99.3% of ^{238}U and 0.7% of ^{235}U. However, in a nuclear reactor, enriched uranium is needed which is uranium where the mass fraction of ^{235}U has been increased. We denote the enrichment as [5]:

$$\tilde{e_a} = \frac{N^{25}}{(N^{25} + N^{28})} \tag{2-16}$$

This expression is known as the atomic enrichment, and from the definition, we can deduced that $1-\tilde{e_a} = N^{28}/(N^{28}+N^{25})$ is the Uranium-238 fraction. We can compute the macroscopic cross section using the enrichment as follows [5]:

$$\Sigma^U = \frac{\rho_U N_0}{\tilde{e_a}235 + (1-\tilde{e_a})238}[\tilde{e_a}\sigma^{25} + (1-\tilde{e_a})\sigma^{28}]$$

Another definition way to defined the enrichment is using the masses:

$$\tilde{e_w} = \frac{M^{25}}{(M^{28} + M^{25})}$$

We can also get the mass fraction for ^{238}U based on the enrichment by $1 - \tilde{e_w} = \frac{M^{28}}{(M^{25}+M^{28})}$. Using this definition to compute the macroscopic cross section:

$$\Sigma^U = \rho N_0 \left[\frac{1}{235}\tilde{e_w}\sigma^{25} + \frac{1}{238}(1-\tilde{e_w})\sigma^{28}\right]$$

There exits a relation between $\tilde{e_a}$ and $\tilde{e_w}$. Using $N^{25} \sim M^{25}/235$ and $N^{28} \sim M^{28}/238$:

$$\tilde{e_a} = \frac{\frac{M^{25}}{235}}{(\frac{M^{25}}{235} + \frac{M^{25}}{235})}$$
$$\tilde{e_a} = \frac{\frac{1}{235}\frac{M^{25}}{M}}{(\frac{1}{235}\frac{M^{25}}{M} + \frac{1}{238}\frac{M^{28}}{M})}$$
$$\text{Using} \tilde{e_w \sim \frac{M^{25}}{M}} \text{and} \tilde{1 - e_w \sim \frac{M^{28}}{M}}$$
$$\tilde{e_a} = \frac{\frac{238}{235}\tilde{e_w}}{(\frac{238}{235})\tilde{e_w} + (1 - \tilde{e_w})}$$

which finally becomes:

$$\tilde{e_a} = \frac{1.0128\tilde{e_w}}{1 + 0.0128\tilde{e_w}}$$

Using the relation for a level $\tilde{e_w} = 0.007$, the atomic enrichment would be $\tilde{e_a} = 0.00709$, and the values gets closer the higher the enrichment. This means that the approximation $\tilde{e_w} \approx \tilde{e_a} \approx \tilde{e}$ is accurate.

2.7. Neutrons Cross Sections

So far, we have only introduced the probability that a neutron interacts with a nucleus but we have not talked about the processes that could happened afterwards. The cross section introduced before is known as the total cross section an is denoted as σ_t. When a neutron hits a nucleus, it is either scatter or absorbed, this could be considered in our relations as [5]:

$$\sigma_f = \sigma_s + \sigma_a$$

In the expression σ_s and σ_a denotes the scattering and absorption cross sections. With this formulation of the total cross section we can easily compute the probability for given interaction to end in scattering or absorption using the fractions σ_s/σ_t and σ_a/σ_t respectively.

However, the scattering cross section is divided further into elastic and inelastic scattering [5]. In the inelastic scattering the neutron give energy to the nucleus leaving it in an excited state. Both kinds of scattering conserve momentum, but only elastic scattering conserve kinetic energy. This arises in the expression:

$$\sigma_s = \sigma_n + \sigma_{n'}$$

Where $\sigma_{n'}$ denotes the cross section for the inelastic scattering. Something similar happens with the absorption scattering.

$$b\sigma_a = \sigma_\gamma + \sigma_f$$

We have two processes, the first one is the formation of a compound nucleus that does not re emit the neutron but eliminates its exited energy via gamma decays, denoted as σ_γ. This process is known as capture reaction and the remaining nucleus could be unstable and decay later on [5]. The other process, more interesting for our application, is a fission process σ_f. We express a particular macroscopic cross section using a sub index $x = s, a, \gamma, f$ which indicates the particular reaction that we are considering.

$$\Sigma_x = N\sigma_x$$

2.7.1. Neutron Energy Range

We have talked about cross sections but we have not considered it energy dependence. In this case, their dependence refers to the energy of the neutron. First we have to establish an upper and a lower limit for the neutron's energy distribution.

- Thermal neutrons: 0.001eV - 1.0 ev
- Intermediate neutrons: 1.0eV - 0.1MeV
- Fast neutrons: 0.1MeV - 10MeV

Neutron produced in a fission reaction follow a energy distribution. If χ(E) is the energy distribution then a reasonable approximation of the distribution [5]:

$$\chi(E) = 0.453 \exp\left(-1.036E\right) \sinh\left(\sqrt{2.29}E\right) \tag{2-17}$$

Prompt neutrons suffer multiple collisions before being absorbed. The nuclei with which they collide follow a thermal distribution with $E_N = \frac{3}{2}kT$, where T is the temperature of the reactor. Therefore, when neutrons collide, they lose energy, passing through an intermediate energy region. Eventually, those neutrons become thermal neutrons, which follow a Maxwell-Boltzmann distribution. These distributions are important because, later in the document, we will see the dependence of cross sections on energy, and this dependence can change the dynamics of the nuclear reactor.

3. The Design of a Nuclear Reactor

Following our study of cross sections and the interactions between nuclei and neutrons, we will now delve into the properties of the nuclear fuel. This chapter will explore the dependence of cross sections on energy, analyze the distributions of neutrons, and estimate the multiplication factor, k.

To achieve this, we will examine how different materials within the reactor core influence reaction rates and the neutron flux distribution across the energy spectrum.

3.1. Nuclear Fuel Properties

Cross sections of fissile and fertile materials are functions of energy; therefore, many of the processes that occur inside a nuclear reactor are determined by the energy of the neutrons. The dependence on energy of the cross sections extends over a broad range from: 10 MeV to 0.001 eV. Fertile materials can undergo fission when absorbing neutrons, but only if the transfer energy surpasses a threshold. A fraction of the total neutrons will be absorbed; this fraction is also energy-dependent. This leads to the following expression:

$$\eta(E) = \frac{\nu \Sigma_f(E)}{\Sigma_a(E)} \tag{3-1}$$

The expression represents the fraction of neutrons that create new neutrons after being absorbed. ν is the number of neutrons produced by fission, and Σ_x represents the cross section of the fission and absorption processes. By definition, Σ depends on the nuclei density, so we can cancel out these factors and end up with σ.

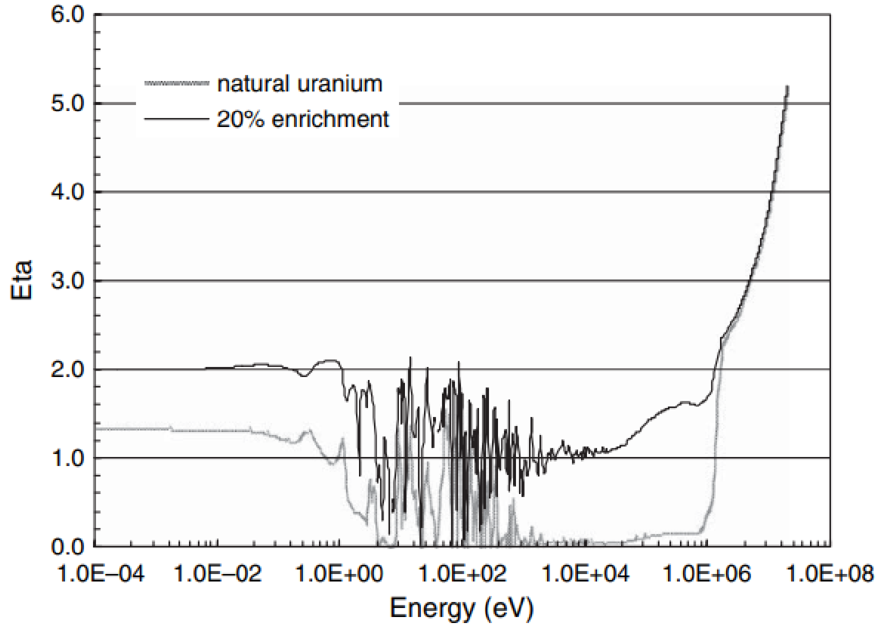

Figure 3-1.: Figure showing two plots of η as function of energy for uranium fuel at different levels of enrichment. Source: [5]

However, nuclear fuel is composed of multiple isotopes, so σ_x should be adjusted to consider the mixture of isotopes. First, we have to consider the enrichment **Eq.**(2-16). We are going to label the cross sections as σ_x^y, where x indicates the process considered (f for fission and a for absorption), and y indicates the fissionable material (fi for fissile and fe for fertile). All of these considerations lead to the following expression:

$$\eta(E) = \frac{\nu\,\tilde{e}\,\sigma_f^{fi}(E) + \nu\,(1-\tilde{e})\,\sigma_f^{fe}(E)}{\tilde{e}\,\sigma_a^{fi}(E) + (1-\tilde{e})\,\sigma_a^{fe}(E)} \tag{3-2}$$

The changes caused by the level of enrichment are reflected on **Fig 3-1**.

Nuclear reactors are designed two concentrate in the fast or thermal energy range, this requirement is due to the valley in the intermediate range of energy. As mentioned before in the document neutrons loss energy when they suffer elastic scattering until they reach thermal equilibrium with the media. There are two types of nuclear reactors, fast and thermal reactors each one with their own specifications.

Fast reactors avoid any kind of material, inside the core, different from fuel so that neutrons

do not experience any scattering and stay in the fast energy range. Low atomic weight materials are capable to to quickly reduce neutrons energy consequently, they are avoid. This effect increases the possibility for uranium-238 to absorb neutrons which leads to an deplete on neutrons [5]. This make impossible for a fast reactor to be fueled with natural uranium [5] and in need of high enrichment uranium $\tilde{e} \gtrsim 10\%$.
The opposite situation happens for thermal reactor. They need materials called moderators to slow-down the neutrons below the valleys in **Eq.**(3-2). When a optimized fuel-moderator is achieved, a thermal nuclear can operate with much lower enrichment [5]. We must examine the properties of a moderator to understand this behaviour.

3.2. Slow Down Decrement

To measure the effectiveness of a nucleus to slow neutrons down by elastic scattering, we use the slow down decrement denoted as ξ. It is defined as the mean value of the logarithm of the fraction energy loss [5]:

$$\xi := \overline{\ln\left(\frac{E}{E}\right)} = \int \ln\left(\frac{E}{E'}\right) p(E \to E')dE' \tag{3-3}$$

A long deduction gives us that:

$$p(E \to E') = \frac{1}{(1-\alpha)E} dE' \tag{3-4}$$

Where $\alpha = \left(\frac{A-1}{A+1}\right)^2$, which can be replaced into **Eq.**(3-3) resulting in:

$$\xi = 1 + \frac{\alpha}{1-\alpha} \ln\alpha \tag{3-5}$$

This parameter can be approximated as $\xi \approx \frac{2}{A+2/3}$. Using this parameter, we can estimate the number of collisions to reduce the energy of a neutron from fast neutrons to thermal neutrons. For instance, consider $E_1, E_2, \ldots, E_n$ to be the neutron energies after the i-th collision, this would be:

$$\ln\left(\frac{E_0}{E_n}\right) = \ln\left(\frac{E_0}{E_1}\right) + \ln\left(\frac{E_1}{E_2}\right) + \cdots + \ln\left(\frac{E_{n-1}}{E_n}\right) \tag{3-6}$$

Replacing each of the terms for the average logarithmic energy loss ξ, we have:

$$n = \frac{1}{\xi}\ln\left(\frac{E_0}{E_n}\right) \tag{3-7}$$

Evaluating the expression for hydrogen, we get $n \approx 18$. However, this expression considers only one nucleus. In order to consider the effects of other isotopes, we have to make an average over their ξ, resulting in:

$$\bar{\xi} = \frac{1}{\Sigma_s}\sum_i \xi_i \Sigma_{si} \tag{3-8}$$

The concept of the slow down decrement is crucial in understanding how neutrons lose energy through collisions. This directly impacts the design and efficiency of neutron moderators, which are essential components in thermal reactors.

3.3. Neutron Moderators

Thermal reactors must reduce the neutrons' energy with as few collisions as possible to transit to the thermal region without being absorbed by the resonances [5]. The slowing down decrement is the parameter most suitable for this purpose.

A good moderator must possess additional properties beyond just a high slowing down decrement. One crucial property is the slowing down power, defined as $\xi\Sigma_s$, where Σ_s is the macroscopic scattering cross section. This parameter indicates the effectiveness of a material in slowing down neutrons through scattering interactions. A high slowing down power ensures that neutrons lose energy efficiently during collisions.

Another important parameter is the slowing down ratio, which is the ratio of the material's slowing down power to its thermal absorption cross section, Σ_a(thermal). This ratio indicates how well a material can slow down neutrons without absorbing them. A high slowing down ratio is desirable because it means the material can effectively moderate neutrons to thermal energies while minimizing neutron absorption.

For example, heavy water (D_2O) has a high slowing down ratio, making it an excellent moderator for reactors using natural uranium fuel. On the other hand, materials with lower slowing down ratios, such as ordinary water (H_2O), require enriched uranium fuel to achieve efficient moderation.

Table 3-1.: Slowing Down Properties of Common Moderators. Source: [5]

Moderator	Slowing Down Decrement ξ	Slowing Down Power $\xi\Sigma_s$	Slowing Down Ratio $\frac{\xi\Sigma_s}{\Sigma_a(\text{thermal})}$
H_2O	0.93	1.28	58
D_2O	0.51	0.18	21,000
C	0.158	0.056	200

3.3.1. Energy Spectra of Neutrons

Having discussed moderation, it is time to study the energy spectra of neutrons. This energy spectrum results from the competition between scattering and absorption reactions.

Neutrons with kinetic energies around the thermal range lose energy during scattering processes. In contrast, thermal neutrons do not lose energy because they are in thermal equilibrium with the medium. When the reactor medium has both a large average energy loss per collision and a high ratio of scattering to absorption cross-sections, neutrons follow a distribution close to thermal equilibrium, known as soft or thermal spectra. Conversely, systems that do not meet these conditions are characterized by a distribution close to the fission spectrum, known as hard or fast spectra.

We can express this distribution in terms of the density distribution $\tilde{n}'''(E)dE$, which is the number of neutrons/cm^3 with energies between E and $E + dE$. However, the neutron flux is more frequently used, defined as:

$$\varphi(E) = v(E)\tilde{n}'''(E) \tag{3-9}$$

where $v(E)$ corresponds to the neutron speed with kinetic energy E. Together with the macroscopic cross-section **Eq.**(2-13), which can be interpreted as the probability of a neutron colliding per cm traveled, we can construct the probability distribution of the number of collisions of type x per cm^3 per second for neutrons with energy between E and $E + dE$ as:

$$\Sigma_x(E)\varphi(E)dE \tag{3-10}$$

Integrating over all energy, we get the probable number of collisions of type x per cm^3 per second of all neutrons [5].

For instance, consider the scenario where a collision removes a neutron, either by absorption or scattering, from the energy region E and $E + dE$. However, neutrons colliding from another energy region, say E' and $E' + dE'$, enter the first region. When the number of neutrons leaving the region and entering it are equal, we have a stationary state [5].

An expression for the balance situation can be deduced by using $\Sigma_t(E) = \Sigma_s(E) + \Sigma_a(E)$ and the probability that a neutron scattered from the energy region $E' + dE'$ ends up in $E + dE$, denoted as $P(E' \to E)$ and $P(E \to E')$. Additionally, we have to consider the prompt neutrons, whose number will be $\chi(E)$ **Eq.**(2-17) multiplied by the number of neutrons produced in each fission, denoted as s_f'''. This results in:

$$\Sigma_t(E)\varphi(E) = \int P(E' \to E)\Sigma_s(E')\varphi(E')dE' + \chi(E)s_f''' \tag{3-11}$$

We already know the distribution of $P(E' \to E)$ from **Eq.**(3-4). The **Eq.**(3-11) is known as the balanced equation. Finally, we can define the parameter $\Sigma_s(E' \to E) = p(E' \to E)\Sigma_s(E')$ for brevity. Now we are going to delve into the three different regions introduced before and, using the balanced equation, deduce the flux.

3.3.2. Fast Neutrons

This energy range is dominated by fission neutrons that have suffered almost no collisions because even one collision can dissipate too much energy. Using this idea, we can approximate the distribution as:

$$\varphi(E) \approx \frac{\chi(E)S_f'''}{\Sigma_t(E)} \tag{3-12}$$

This distribution is deformed by inelastic interactions and absorption processes. In fast reactors, neutrons are absorbed before they experience many collisions and pass the low-energy tail of the distribution.

3.3.3. Intermediate Neutrons

Having talk about the upper energy range in the distribution of neutrons, we must explored the range where the thermal motion of nuclei must be considered in our calculation.
Before delve into this distribution we have to introduce the concept of slowing-down density denoted as $q(E)$ [5].

Slowing Down Density

The slowing-down density defined as the number of neutrons slowing down past energy E per cm^3 per second [5].
In energies around $1.0eV$ neutrons can gain energy through collisions with the medium [8]. Every fission neutron produced over the energy range $1.0eV - 0.1MeV$ will arrive to this range if it is not absorbed. This fact can be expressed as:
We can express the source term $q(E)$ as follows:

$$q(E) = \underbrace{\int_E^{\infty} \chi(E')s_f'''dE'}_{\text{Term 1}} - \underbrace{\int_E^{\infty} \Sigma_a(E')\varphi(E')dE'}_{\text{Term 2}} \tag{3-13}$$

Here, term 1 represents the contribution from the fission produced about the energy E, and term 2 represents the neutrons absorbed before arriving to $< E$. We can make the following approximation $\chi(E) \approx 0$ for $E < 0.1MeV$, then the following approximation is accurate $\int_E^\infty \chi(E')dE' \approx \int_0^\infty \chi(E')dE' = 1$. This leads to the following approximation of $q(E)$:

$$q(E) \approx s_f''' - \int_E^\infty \Sigma_a(E')\varphi(E')dE'$$

By taking the derivative of the expression we end up with $\frac{d}{dE}q(E) = -\Sigma_a(E)\varphi(E)$. This means that an increase in $\Sigma_a(E)$ causes a decrease in the slowing down density. In the intermediate region most of the contribution to absorption comes from resonances. Additionally, cross section between resonances are small enough to be ignored [5]. Finally, we are below the energy range where fission neutrons are produced, then we can simplify **Eq.**(3-11) to :

$$\Sigma_s(E)\varphi(E) = \int_E^{E/\alpha} p(E' \to E)\Sigma_s(E')\varphi(E')dE' \tag{3-14}$$

By solving the integral equation, we can establish the relation $\Sigma_s(E)\varphi(E) = \frac{C}{E}$. Since we are interested in the neutrons that will scattered in the interval $\alpha\, E'' \leq$, we will consider only with initial energy between $E < E' < E/\alpha$. Considering this we can end up with the following expression for q:

$$q = \int_E^{E/\alpha} \left[\int_{\alpha\, E'}^{E} \frac{1}{(1-\alpha)E'} \frac{C}{E} dE'' \right] dE'$$

Solving the integral we end up with:

$$q(E) = \underbrace{\left[1 + \frac{\alpha}{1-\alpha} \ln \alpha \right]}_{\text{Term 1}} C$$

The similarity of the first term 1 to ξ in **Eq.**(3-5) is noticeable. Using this result and the solution for **Eq.**(3-14) we get and expression for φ:

$$\varphi(E) \approx \frac{q(E)}{\xi\, \Sigma_s(E)E} \tag{3-15}$$

Once again, we can improve this expression to consider multiple isotopes and materials by using **Eq.**(3-8).

3.3.4. Thermal Neutrons

After some time and several collisions, the energy of neutrons will drop below 0.1, eV. At this point, further collisions may either absorb or release energy. Something after this, neutrons reach thermal equilibrium with the medium at, say, temperature T which is the one of the reactor. In this region of energy the term related to fission neutrons in **Eq.**(3-11) vanishes [5]. A first approximation is to consider that the neutron flux follows Maxwell-Boltzmann distribution:

$$\varphi(E) \approx \varphi_{MB}(E) = \frac{1}{(kT)^2} \exp(-E/(kT)) \tag{3-16}$$

However, the scenario is not that simple, as many neutrons are absorbed before reaching thermal equilibrium. Consequently, thermal neutrons do not follow a Maxwell-Boltzmann distribution, as their distribution is shifted towards higher energies. Describing these circumstances is not an easy task, since neutrons collide with atoms or even the lattice of the material rather than with nuclei, complicating the calculations [8].
An approximation is to use a Maxwell-Boltzmann distribution but with an effective temperature $T_k > T$:

$$\begin{aligned} \varphi(E) &\approx \varphi_{MB}(E; T_k) \\ T_k &= T + a\left(\frac{\Sigma_a}{\xi \Sigma_s}\right) \end{aligned} \tag{3-17}$$

Where a is a fitted constant.

3.4. Reaction Rates Averaged Over Energy

The ability to sustain a chain reaction greatly depends on the distribution of neutrons across the energy range, which in turn depends on the composition of the different materials in the core and their effectiveness in slowing down neutrons [5]. For this reason, cross sections must be averaged over the entire energy spectrum. We define the average cross section as:

$$\bar{\Sigma}_x = \int_0^\infty \Sigma_x(E)\varphi(E)\,dE \Big/ \int_0^\infty \varphi(E)\,dE \tag{3-18}$$

From the definition of Σ_x in **Eq.**(2-13), it is possible to use σ by canceling the atom density. The flux can be expressed as the product of the mean speed and the density of neutrons:

$$\phi = \bar{v}n''' \tag{3-19}$$

From this relation, the mean velocity can be defined as:

$$\bar{v} = \int_0^\infty v(E)\tilde{n}'''(E)\,dE \Big/ \int_0^\infty \tilde{n}'''(E)\,dE \tag{3-20}$$

A more precise treatment of neutron populations requires cross section averaging over specific energy ranges rather than the entire energy spectrum [5]. The reaction rates should be partitioned as:

$$\int \sigma_x(E)\varphi(E)\,dE = \int_T \sigma_x(E)\varphi(E)\,dE + \int_I \sigma_x(E)\varphi(E)\,dE + \int_F \sigma_x(E)\varphi(E)\,dE \tag{3-21}$$

Here, T denotes the thermal region ($0 \leq E \leq 1.0\,\mathrm{eV}$), I denotes the intermediate or resonance region ($1.0\,\mathrm{eV} \leq E \leq 0.1\,\mathrm{MeV}$), and F denotes the fast region ($0.1\,\mathrm{MeV} \leq E \leq \infty$). This can be written as the sum of each averaged energy:

$$\bar{\sigma}_x\phi = \bar{\sigma}_{xT}\phi_T + \bar{\sigma}_{xI}\phi_I + \bar{\sigma}_{xF}\phi_F$$

This expression is obtained by multiplying and dividing **Eq.**(3-21) by:

$$\phi_\Omega = \int_\Omega \varphi(E)\,dE, \quad \Omega = \mathrm{T,\ I,\ F}$$

Defining the energy-averaged cross section as:

$$\bar{\sigma}_{x\Omega} = \int_{\Omega} \sigma_x(E)\varphi(E)\, dE \Big/ \int_{\Omega} \varphi(E)\, dE, \quad \Omega = \text{T, I, F} \tag{3-22}$$

More advanced approximations, known as multi-group methods, divide the spectrum into more than three intervals.

3.5. Multiplicative Factor for Infinite Media

This discussion introduces the concept of the infinite multiplication factor k_∞, which is defined by the multiplication factor **Eq.**(2-9) for an infinite reactor approximation. The term "infinite" refers to the assumption of an infinite medium, additionally it is assumed that all neutrons are generated instantaneously.
To account for the finite volume of the reactor, we introduce the non-leakage probability:

$$k = k_\infty P_{NL} \tag{3-23}$$

Here, P_{NL} is the probability that a neutron does not leak from the reactor before being absorbed. This factor depends on the geometry, the volume of the core, the distribution, and the composition of the materials within the reactor [5].
An expression for k_∞, derived from the definition and using energy-averaged cross sections and flux given in the previous section, is:

$$k_\infty = \nu \bar{\Sigma}_f \big/ \bar{\Sigma}_a \tag{3-24}$$

It is crucial to note that only fissionable materials contribute to $\bar{\Sigma}_f$, while $\bar{\Sigma}_a$ considers all the materials composing the reactor core [5].
In the next chapter, we will delve deeper into the study of this parameter and ultimately determine the equations that describe the behavior of a reactor.

4. Structure of a Nuclear Reactor

When designing a power reactor core, two key criteria must be satisfied. First, criticality must be sustained across the entire range of power levels and throughout the fuel depletion process. Second, the core must allow for efficient transfer of the thermal energy produced by fission reactions without causing overheating [5]. In this chapter, we will discuss neutron behavior and the influence of the reactor lattice on the multiplication factor.

4.1. Time Dependence of Neutron Flux

In the previous chapter, we examined neutron flux but disregarded its time dependence. To investigate this aspect, we will analyze two types of systems:

- Non-multiplicative systems: Systems without fissionable material.
- Multiplicative systems: Systems containing fissionable material.

To perform the necessary calculations, we must define the following variables:

- $n(t)$: The total number of neutrons at a given time t.
- $\bar{v}$: The average velocity of neutrons.
- Σ_x: The macroscopic cross-section for a specific reaction x (e.g., absorption, scattering, or fission).

4.1.1. Infinite Multiplicative Media

In this initial approximation, we will account only for the effects of prompt neutrons and neutron leakage. Based on these assumptions, we can outline the factors contributing to the rate of change in the neutron population over time [5]:

$$\frac{d}{dt}n(t) = \text{neutrons produced per second by the source} + \text{neutrons produced by fission} \\ - \text{neutrons absorbed}$$

To represent the neutrons introduced by an external source, we define the variable $S(t)$, which describes the rate of neutron production by the source at time t [5]. In addition, let ν be the average number of neutrons, thus $\nu\Sigma_f\bar{v}n(t)$ is the number of fission neutrons produced per second. Finally, $\Sigma_a\bar{v}n(t)$ is the number of neutrons absorbed per second. With this we get the expression:

$$\frac{d}{dt}n(t) = S(t) + \nu\Sigma_f\bar{v}n(t) - \Sigma_a\bar{v}n(t) \tag{4-1}$$

It can be easily shown that the mean lifetime of a neutron, defined as the time between its production and absorption, is given by $l_\infty = \frac{1}{\bar{v}\Sigma_a}$. By using the definition of k_∞ from **Eq.**(3-23), we obtain the following equation for the time dependence of the neutron population:

$$\frac{d}{dt}n(t) = S(t) + \frac{(k_\infty - 1)}{l_\infty}n(t) \tag{4-2}$$

If there is no external source and neutrons are produced solely through fission ($S(t) = 0$), the equation simplifies to:

$$\frac{d}{dt}n(t) = \frac{(k_\infty - 1)}{l_\infty}n(t)$$

This equation describes three possible behaviors for the neutron population, depending on the value of k_∞:

- $k_\infty < 1$: The neutron population decreases exponentially, indicating a sub critical state.
- $k_\infty > 1$: The neutron population increases exponentially, corresponding to a supercritical state.
- $k_\infty = 1$: The neutron population remains constant, representing a critical state.

4.1.2. Finite Multiplicative Media

In real life nuclear reactors are finite, thus neutrons could escape through the borders of the reactor. This effect should be considered in the rate of change in the neutrons populations:

$$\begin{aligned}\frac{d}{dt}n(t) = &\text{ neutrons produced per second by the source} + \text{neutrons produced by fission}\\ &-\text{neutrons absorbed} - \text{neutrons escaping the system}\end{aligned}$$

First, it is important to notice that the effect of the leakage of neutrons is proportional to neutrons population at a time t [5]. Define the coefficient Γ in a way that:

$$\text{Neutrons escaping the system} = \Gamma\Sigma_a\bar{v}n(t)$$

This leads to:

$$\frac{d}{dt}n(t) = S(t) + \nu\Sigma_f\bar{v}n(t) - \Sigma_a\bar{v}n(t) - \Gamma\Sigma_a\bar{v}n(t) \tag{4-3}$$

From the definition of Γ, we can deduce expressions for the leakage probability (P_L) and the non-leakage probability (P_{NL}). The non-leakage probability corresponds to neutrons that remain inside the reactor and can induce new fissions. We define the leakage probability as $P_L = \frac{\text{neutrons that escape}}{\text{neutrons produced}}$, which gives the following expression [5]:

$$P_L = \frac{\Gamma\Sigma_a\bar{v}n}{\Sigma_a\bar{v}n + \Gamma\Sigma_a\bar{v}n} = \frac{\Gamma}{1+\Gamma}$$

The non-leakage probability P_{NL} can be easily derived from the definition of P_L as:

$$P_{NL} = \frac{1}{1+\Gamma} \tag{4-4}$$

In the next section, we will explore the relationship between the size and shape of the reactor and the parameter Γ. For now, we can rewrite **Eq.**(4-3) in terms of P_{NL} as follows:

$$P_{NL}\frac{d}{dt}n(t) = P_{NL}S(t) + \frac{(P_{NL}k_\infty - 1)}{l_\infty}n(t)$$

By defining $k = k_\infty P_{NL}$ and $l = l_\infty P_{NL}$, and substituting these into the above equation, we obtain:

$$\frac{d}{dt}n(t) = S(t) + \frac{(k-1)}{l}n(t) \tag{4-5}$$

4.1.3. Delayed Neutron Kinetics

Around 99% of fission neutrons are prompt neutrons, emitted immediately at the moment of fission [5]. The remaining fraction, denoted by β, are delayed neutrons emitted through the decay of fission products. The nuclei that emits the delayed neutrons is divided in six groups based on their half-lives which go from fraction of a second to nearly a minute [5]. These groups are showed in the table **4-1**.

We defined β as the sum of the delayed neutrons fraction of each group, this is:

$$\beta = \sum_{i=1}^{6} \beta_i \tag{4-6}$$

For instance consider the half-life for the ith group by $t_{i1/2}$. Using these half-lives we can define the average half-life of the delayed neutrons by :

$$t_{1/2} = \frac{1}{\beta}\sum_{i=1}^{6} \beta_i t_{i1/2}$$

Table 4-1.: Delayed Neutron Fractions for Different Isotopes. Source: [5]

Approximate Half-life (sec)	U^{233}	U^{235}	Pu^{239}
56	0.00023	0.00021	0.00007
23	0.00078	0.00142	0.00063
6.2	0.00064	0.00128	0.00044
2.3	0.00074	0.00257	0.00069
0.61	0.00014	0.00075	0.00018
0.23	0.00008	0.00027	0.00009
Total delayed fraction	0.00261	0.00650	0.00210
Total neutrons/fission	2.50	2.43	2.90

Since half-lives and decay constant are related by $t_{i1/2} = 0.693/\lambda_i$, it is possible to define the average decay constant by :

$$\frac{1}{\lambda} = \frac{1}{\beta}\sum_{i=1}^{6}\beta_i\frac{1}{\lambda_i} \tag{4-7}$$

Until now, the mean lifetimes l and l_∞ have only considered prompt neutrons. To account for the contributions of delayed neutrons, denoted by l_d, we must derive an expression for their lifetime:

$$l_d = \underbrace{l}_{\text{Term 1}} + \underbrace{\frac{1}{\lambda}}_{\text{Term 2}} \tag{4-8}$$

The first term represents the time it takes for a delayed neutron to be absorbed or escape, while the second term accounts for the time between the fission of the parent nucleus and the emission of the delayed neutron through the decay of fission products.

Taking both prompt and delayed neutrons into account, the average neutron lifetime is defined as:

$$\bar{l} = (1-\beta)l + \beta l_d = l + \frac{\beta}{\lambda} \tag{4-9}$$

It is evident that $\bar{l} >> l$. The presence of delayed neutrons significantly increases the mean neutron lifetime, leading to modifications to the equations for the rate of change in neutron population, such as equation (4-3), due to the substantial delays involved.

4.1.4. Kinetic Equations

To incorporate the effects of delayed neutrons into the neutron balance equation (4-3), we separate the contributions from prompt and delayed neutrons. Defining the fraction of delayed neutrons as β, the prompt neutrons are produced at a rate $(1-\beta)\nu\Sigma_f\bar{v}n(t)$ [5]. The delayed neutrons, on the other hand, are produced by the decay of fission products. Let $C_i(t)$ represent the number of precursor nuclei producing neutrons with a half-life $t_{i1/2}$. Thus, the production rate of delayed neutrons is $\lambda_i C_i(t)$. The resulting expression for the neutron population balance is as follows:

$$\frac{d}{dt}n(t) = S(t) + (1-\beta)\nu\Sigma_f\bar{v}n(t) + \sum_i \lambda_i C_i(t) - \Sigma_a\bar{v}n(t) - \Gamma\bar{v}n(t) \tag{4-10}$$

Since the concentration of the precursors is unknown we required extra equations to determine their concentrations. Since we divided the delayed group in six we are going to have six different equations, each one with the form of a balance equation [5]:

$$\frac{d}{dt}C_i(t) = \text{precursors produced per second} - \text{precursors decaying per second}$$

Since the number of precursors produced per second is $\beta_i\nu\Sigma_f\bar{v}n(t)$ while the decay rate is $\lambda_i C_i(t)$. This leads to:

$$\frac{d}{dt}C_i(t) = \beta_i\nu\Sigma_f\bar{v}n(t) - \lambda_i C_i \qquad i = 1,2,3,...,6 \tag{4-11}$$

Reactivity

Define the reactivity as:

$$\rho = \frac{k-1}{k} \tag{4-12}$$

The reactivity can have three possible conditions:

$$\rho = \begin{cases} > 0 & \text{(supercritical)} \\ = 0 & \text{(critical)} \\ < 0 & \text{(subcritical)} \end{cases}$$

Additionally, define the prompt generation time as $\Lambda = 1/k$ with these definitions the kinetics equations (4-10) and (4-11) can be simplified as:

$$\frac{d}{dt}n(t) = S(t) + \frac{(\rho-\beta)}{\Lambda}n(t) + \sum_i \lambda_i C_i(t) \tag{4-13}$$

$$\frac{d}{dt}C_i(t) = \frac{\beta_i}{\Lambda}n(t) - \lambda_i C_i(t), \qquad i = 1, 2, \ldots, 6 \tag{4-14}$$

4.2. Spatial Diffusion of Neutrons

We have include the diffusion of neutrons by introducing the factor P_{NL}. However a better understanding of the relation between P_{NL}, the shape and size of a nuclear reactor is necessary to understand how these parameters affects the reactivity.

4.2.1. Continuity Equation

Consider an arbitrary volume V centered at $\vec{r} = (x, y, z)$, and establish a balance equation between the number of neutrons leaving and entering V [2]:

$$\text{Neutrons leaking from } V + \text{ Neutrons absorbed inside } V =$$
$$\text{Neutrons emitted by a source inside } V + \text{ Neutrons produced by fission inside } V$$

Neutrons Leaking

Neutrons pass through the surface of the volume. To describe this, we define $\vec{J} = J(x, y, z)$ as the current density per cm^2. If J_i represents the neutron current along the $j-k$ plane, then:

$$\textbf{Neutrons leaking} = \sum_{i=x}^{z} \left[J_i \left(i + \frac{1}{2}di, \cdots \right) - J_i \left(i - \frac{1}{2}di, \cdots \right) \right] \frac{1}{di}$$

This can be expressed as:

$$\textbf{Neutrons leaking} = \int_V (\nabla \cdot \vec{J})\, dV \tag{4-15}$$

Neutrons Absorbed

The number of neutrons absorbed is given by $\Sigma_a \Phi$ [2], where Φ is the neutron flux defined as $\Phi = \bar{v}n'''$. Thus:

$$\textbf{Neutrons absorbed} = \int_V \Sigma_a \Phi\, dV \tag{4-16}$$

Here, n''' is averaged over all energy ranges: $\bar{n'''} = \int_0^\infty n'''(E)\, dE$. Additionally, $\Phi = \Phi(E, \vec{r})$ can be expressed as $\phi(\vec{r}) = \int_0^\infty \phi(E, \vec{r}) dE$ with this change the flux depends on $\vec{r}$ [2].

Neutrons Produced by a Source

Let $S'''(\vec{r})$ represent the number of neutrons produced by a source per second per unit volume. The total number of neutrons produced inside V is:

$$\textbf{Neutrons produced by a source} = \int_V S'''\, dV \tag{4-17}$$

Neutrons Produced by Fission

The total number of neutrons produced by fission inside V is given by:

$$\textbf{Neutrons produced by fission} = \int_V \nu\Sigma_f \Phi \, dV \tag{4-18}$$

Balance Equation

Since all the terms introduced are integrated over the same volume, in the equation (4-19) the integral vanishes. In a stationary state, where the neutron population remains constant over time ($\partial n/\partial t = 0$), the continuity equation becomes:

$$\nabla \cdot \vec{J} + \Sigma_a(\vec{r})\phi(\vec{r}) = S'''(\vec{r}) + \nu\Sigma_f(\vec{r})\phi(\vec{r}) \tag{4-19}$$

However, in the equation we got two unknowns variables, $\vec{J}$ and ϕ, this forces us to express $\nabla \cdot \vec{J}$ in terms of ϕ. In order to solve this situation, we will use the diffusion approximation along with Fick's Law [2].

4.2.2. Diffusion approximation

Fick's law is the start point of diffusion theory [2]. Fick's law states that if the concentration of a solute is grater in one region of a solution than in another, the solute diffuses from the region of higher concentration to the region of lower concentration. Moreover, the rate of solute flow is proportional to the negative of the gradient of the solute concentration [2]. A good approximation is to assume that neutrons inside a reactor behave mostly as a solute in a solution, this is:

$$\vec{J} = -D(\vec{r})\nabla\phi \tag{4-20}$$

Where D denotes the diffusion coefficient. Some approximations defined $D(\vec{r}) = 1/\,3\Sigma_{tr}$, where Σ_{tr} is the transport cross sections an is defined as $\Sigma_{tr} = \Sigma_t - \bar{\mu}\Sigma_s$, $\bar{\mu}$ is the average scattering angle. For isotropic scattering $\bar{\mu} = 0$, this reduces the transport cross section to the total cross section Σ_t [5].

Using Fick's law in equation (4-19) yields the neutron diffusion equation [5]:

$$-\nabla \cdot D(\vec{r})\nabla\phi + \Sigma_a(\vec{r})\phi(\vec{r}) = S'''(\vec{r}) + \nu\Sigma_f(\vec{r})\phi(\vec{r}) \tag{4-21}$$

4.2.3. Boundary Conditions

It is easy to notice that the diffusion equation is a second order equation. This means that, for example in one dimensional problems, two arbitrary constants raises from the solution. In order to know the value of these constants two boundary conditions must be known. An easy way to determinate these conditions is to used what is known as partial current currents [5]. To understand the partial currents, let $J_x(x)$ be the net number of neutrons crossing the plane $y - z$ per second per cm^2. Now we factorize $J_x(x)$ in two different contributions: $J_x^+(x)$ and $J_x^-(x)$ traveling in the positive and negative x directions, respectively [5]. This is:

$$J_x = J_x^+(x) - J_x^-(x)$$

It can be shown that in the diffusion approximation:

$$J_x^{\pm}(x) = \frac{1}{4}\phi(x) \pm \frac{1}{2}J_x(x)$$

Employing (4-20) the equation yields:

$$J_x^{\pm}(x) = \frac{1}{4}\phi(x) \pm \frac{1}{2}D(r)\frac{d}{dx}\phi(x)$$

We can define the boundaries of this surface as x_r and x_l. In this case, imagine a surface that does not allow any neutrons to enter, which could occur if a vacuum extends infinitely without any neutron sources. This scenario is known as a vacuum boundary condition.

If the boundary is located at x_l, the neutron current condition can be expressed as $J_x^+(x_l) = 0$. Conversely, for a boundary at x_r, the condition would be $J_x^-(x_r) = 0$. Using the definition of the partial current, we can write the condition for the right boundary as:

$$0 = \frac{1}{4}\phi(x_r) - \frac{1}{2}D \left| \frac{d}{dx}\phi(x) \right|_{x_r}$$

Furthermore, in the context of isotropic scattering, the diffusion coefficient is defined as $D = \frac{1}{3\Sigma_t}$, while the mean free path λ is given by $\lambda = \frac{1}{\Sigma_t}$. This allows us to reformulate the vacuum boundary condition as follows:

$$\frac{\phi(x_r)}{\left| \frac{d}{dx}\phi(x) \right|_{x_r}} = \frac{2}{3}\lambda$$

Let $d = \frac{2}{3}\lambda \approx 0.66\lambda$. Frequently, when vacuum boundaries are encountered, the most straightforward approach is to apply the zero-flux condition and adjust the dimensions accordingly. This is expressed as $\phi(x_r + d) = 0$ and $\phi(x_l + d) = 0$. We refer to these conditions as the extrapolated boundaries, denoted by $\tilde{x_r}$ and $\tilde{x_l}$.

A more accurate approach, based on transport theory, yields a value of $d_{tr} = 0.7104\lambda$. This concept is illustrated in Figure **4-1**.

4.3. Non-Leakage Probability

Finally, to determine the non-leakage probability lets consider a multiplicative system ($\nu\Sigma_f > 0$) and a uniform system which means the source $S'''(r) = S_0'''$, $D(\vec{r}) = D = cte$ and all cross section are space-independent constants. Additionally, let $L = \sqrt{D/\Sigma_a}$ and k_∞ as in equation (3-24). Including all of these in the diffusion equation (4-21) yields:

$$-\nabla^2\phi(\vec{r}) + \frac{1}{L^2}\phi(\vec{r}) = \frac{1}{D}s_0''' + \frac{1}{L^2}k_\infty\phi(\vec{r}) \tag{4-22}$$

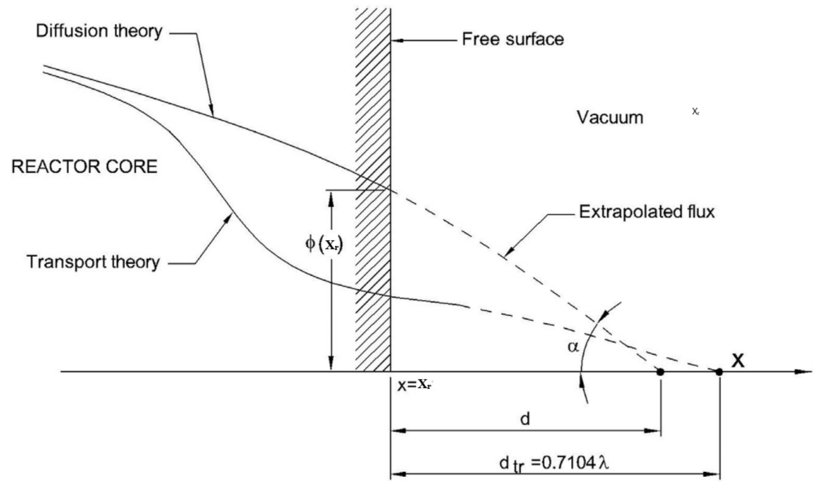

Figure 4-1.: Extrapolated boundary conditions. Source: [12]

4.3.1. Spherical Geometry

In spherical geometry, the Laplacian ∇^2 is replaced by:

$$-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi}{dr}\right)+\frac{1}{L^2}(1-k_\infty)\phi=\frac{1}{D}S_0'''$$

The solution to this equation is a superposition of the general and particular solutions, $\phi(r)=\phi_g(r)+\phi_p(r)$. Assuming a uniform source, we have $\phi_p(r)=\text{const}=\frac{S_0'''}{(1-k_\infty)\Sigma_a}$ [5]. For the general solution, consider the case where $k_\infty<1$. The equation becomes:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi_g}{dr}\right)-\frac{1}{L^2}(1-k_\infty)\phi_g=0$$

Applying the previously discussed boundary conditions, the solution is:

$$\phi(r)=\frac{S_0'''}{(1-k_\infty)\Sigma_a}\left[1-\frac{\tilde{R}\sinh(\kappa r)}{r\sinh(\kappa\tilde{R})}\right]$$

where $\kappa=\frac{1}{L}\sqrt{1-k_\infty}$ and $\tilde{R}=R+\frac{2}{3}\lambda$, representing the extrapolated boundary conditions.

Now consider the supercritical case $k_\infty > 1$, where the particular solution is:

$$\phi_p = -\frac{S_0'''}{(k_\infty - 1)\Sigma_a}$$

Solving the general equation and applying the boundary conditions, the solution is:

$$\phi(r) = \frac{S_0'''}{(k_\infty - 1)\Sigma_a}\left[\frac{\tilde{R}\sin(Br)}{r\sin(B\tilde{R})} - 1\right]$$

where $B = \frac{1}{L}\sqrt{k_\infty - 1}$.

Criticality Condition

In the supercritical solution, consider the limit $\lim_{B\tilde{R}\to\pi} \phi_p \to \infty$, implying that the sphere becomes critical [5]. The condition for criticality is then:

$$\frac{1}{L}\sqrt{k_\infty - 1}\tilde{R} = \pi$$

Solving for k_∞ gives:

$$k_\infty = 1 + \frac{\pi^2 L^2}{\tilde{R}^2}$$

For a finite reactor, the criticality condition is $k = P_{NL}k_\infty = 1$. Thus, for the critical sphere, the non-leakage probability is:

$$P_{NL} = \frac{1}{1 + \left(\frac{\pi L}{\tilde{R}}\right)^2} \tag{4-23}$$

Now lets define two new variables. First, the material buckling defined as $B_m = \frac{1}{L}\sqrt{k_{\infty - 1}}$ and secondly the geometrical buckling $B_g = \pi/\tilde{R}$. With this the criticality condition can be expressed as:

$$B_m = B_g$$

4.3.2. Time-Independent Diffusion Equation

If we set the source to be zero, then the steady diffusion equation (4-21) becomes:

$$\nabla \cdot D(\vec{r})\nabla\phi(\vec{r}) + \nu\Sigma_f\phi(\vec{r}) - \Sigma_a\phi(\vec{r}) = 0 \tag{4-24}$$

In this equation, ϕ tends to zero if the reactor is subcritical. Conversely, if the reactor is in a supercritical state, ϕ tends to infinity. In either case, the kinetic equations (4-10) and (4-11) are necessary to describe the system's behavior [5]. The challenge is to determine the critical state by varying the reactor's geometry or its material composition [5].

To compute this, we apply the following approach: suppose it is possible to adjust the average number of neutrons produced per fission (ν) by a factor ν_0/ν, where ν_0 is the number of neutrons per fission required to bring the reactor to a critical state [5]. Since $k \sim \nu$, we have $\nu_0/\nu = 1/k$ [5]. Thus, the time-independent diffusion equation (4-24) can be rewritten as:

$$\nabla \cdot D(\vec{r})\nabla\phi(\vec{r}) + \frac{1}{k}\nu\Sigma_f\phi(\vec{r}) - \Sigma_a\phi(\vec{r}) = 0 \tag{4-25}$$

It is easy to see that if $\nu_0 > \nu$, then the reactor is subcritical. On the other hand, if $\nu_0 < \nu$, the reactor is supercritical. By incorporating this adjustment into the diffusion equation and solving for k, we transform the problem into finding how far a given configuration (defined by the reactor core's dimensions and cross-sections) is from criticality.

This can be framed as an eigenvalue problem, where k is the eigenvalue and ϕ is the eigenfunction. Typically, these problems have an infinite set of solutions. However, by applying the boundary conditions and focusing on physically meaningful solutions, those in which the neutron flux is positive everywhere within the reactor, we narrow the problem to the relevant solution. This solution corresponds to the largest eigenvalue, the corresponding eigenfuntion ϕ is refered as the fundamental mode solution.

Uniform Reactors

Now suppose that the reactor is uniform, which implies that D is constant. Using the same definitions for k_∞ and L^2 as in equation (4-22), the diffusion equation (4-25) can be written as:

$$\nabla^2\phi + \frac{k_\infty/k - 1}{L^2}\phi = 0$$

Since the term multiplying ϕ is constant, we define $B^2 = \frac{k_\infty/k-1}{L^2}$. From this equation, it can be shown that the non-leakage probability P_{NL} is:

$$P_{NL} = \frac{1}{1+(LB)^2}$$

Here, B is referred to as the geometric buckling, or simply the buckling [5]. To determine the buckling, we must solve the following equation, which is the Helmholtz equation:

$$\nabla^2\phi + B^2\phi = 0 \tag{4-26}$$

The solution must satisfy the condition $0 < \phi < \infty$ within the reactor, as well as the boundary conditions at the reactor's surfaces [5].

4.3.3. Cylindrical Reactor

Given a cylindrical reactor with an extrapolated radius $\tilde{R} = R + \frac{2}{3}\lambda$ and height $\tilde{H} = H + \frac{4}{3}\lambda$, we now examine the buckling. Replacing ∇^2 in equation (4-26) with its form in cylindrical coordinates gives:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{d\phi}{dr}\right) + \frac{\partial^2}{\partial z^2}\phi + B^2\phi = 0$$

This equation corresponds to a partial differential equation that can be solved by separating variables. Assuming the solution takes the form $\phi(r,z) = \psi(r)\chi(z)$, substituting and dividing by ϕ yields:

$$\frac{1}{\psi}\frac{d}{dr}\left(r\frac{d\psi}{dr}\right) + \frac{1}{\chi}\frac{d^2\chi}{dz^2} + B^2 = 0$$

Since B^2 is a constant, the first term depends only on r, and the second term depends only on z, meaning each term must equal a constant for the equation to have a solution. Thus, we assume that the total buckling can be written as $B_r^2 + B_z^2 = B^2$. These constants must satisfy the following differential equations:

$$\begin{aligned} \frac{d}{dr}\left(r\frac{d\psi}{dr}\right) + B_r^2\psi = 0 \\ \frac{d^2\chi}{dz^2} + B_z^2\chi = 0 \end{aligned}$$

Solving these equations gives the expressions $B_z = \pi/\tilde{H}$ and $B_r = 2.405/\tilde{R}$. Thus, the total buckling is:

$$B^2 = \left(\frac{2.405}{\tilde{R}}\right)^2 + \left(\frac{\pi}{\tilde{H}}\right)^2 \tag{4-27}$$

Although spherical reactors are the most efficient due to their higher non-leakage probability (P_{NL}), they represent significant technical challenges, such as structural complexity and cooling issues [8]. This is why most commercial reactors have cylindrical geometry.

In the next chapter, we will explore the different fuels used in reactors, examining how they are managed before, during, and after reactor operation.

5. Nuclear fuel cycles

Now we will examine the life cycle of the materials used as fuel in nuclear reactors. The fuel cycle spans from the mining of the ore to the fabrication of the fuel, its irradiation in the reactor, and the subsequent processing of the spent nuclear fuel [13]. The nuclear fuel cycle can vary depending on several factors, such as:

- The fissile nuclei being used for energy generation, such as any of the isotopes mentioned in **Section** 2.3.
- The form in which the fuel is utilized.
- The type of reactor in which the fuel is deployed.

The nuclear fuel cycle begins with uranium mining and ends with the disposal of nuclear waste [13], although some steps may not apply to every fuel cycle.

5.1. Frontend of Fuel Cycle

The steps involving mining, milling, conversion, enrichment, and fuel fabrication correspond to the "frontend" of the nuclear fuel cycle. Uranium-rich minerals are radioactive primarily due to the daughter products derived from radioactive decays of uranium. In 2019, global uranium production was approximately 54,750 tons, with most of the mined uranium being used as fuel for nuclear power plants [13].

Uranium recovery is achieved through extraction from ores, followed by concentration and purification. This process involves both excavation and in-situ leaching (ISL). Typically, open-pit mining is used for deposits near the surface, while underground mining is applied for deeper deposits [13]. The mined uranium ore is then processed by grinding, followed by uranium leaching using either alkaline or acidic methods. The milling process yields "yellowcake", which contains uranium in the form of U_3O_8, with a uranium content greater than 80% [13].

Approximately 200 tons of U_3O_8 are required to fuel a 1000 MWe nuclear power reactor for one year. The U_3O_8 produced from the uranium mill is further enriched to increase the U^{235} content from 0.72% to between 3% and 5%, which is required for light water reactors. The enrichment process involves converting uranium into uranium hexafluoride (UF_6), which is solid at room temperature but sublimates at 56.5°C, allowing it to be used in isotope separation.

The primary method used for isotope enrichment today is centrifugation, where thousands of rapidly spinning vertical tubes exploit the small mass difference between the uranium isotopes' hexafluorides, leading to their separation [13].

However the UF_6 is not suitable to be used as fuel in a nuclear reactors, hence needs to be converted to ceramic pellets of UO_2 sintered at temperatures over the $1400°C$. Other pallets composed by a mixed of U, Pu oxide (MOX) are fabricated [13]. Currently, conventional UOX fuel have an additive less than 10% of thorium . This increases the thermal distribution by reducing the need of poison in the reactor [14].

5.2. Backend of Fuel Cycle

The processes that occur after the discharge of irradiated fuel from the reactor, such as the temporary storage of spent fuel, reprocessing, and waste management, are collectively known as the "backend" of the nuclear fuel cycle. The energy realised by fission extracted from the fuel is measured as the "burn up" [13]. The most commonly used metric for fuel burn-up is the amount of fission energy produced per unit mass of fuel. This is expressed as the total energy released, measured in megawatt-days, divided by the initial mass of fuel, including both fissile and fertile materials, and is referred to as *megawatt-days per ton* (MWd/T) [15]. Since natural uranium contains only0.72% of the fissile isotope ^{235}U, the burn-up of fuel based on natural uranium is expected to be below $0.72atom\%$. However, due to the breading of ^{239}Pu from neutron absorption in ^{238}U, burn-up can achieve values of up to 1atom% ($10,000 MWd/T$) [13]. In typical pressurized heavy water reactors (PHWRs), the burn-up level is around $7000 MWd/T$. For light water reactors (LWRs) using enriched uranium, burn-up levels can reach 6–7atom%, while in fast reactors, burn-up can exceed 10atom%. In some cases, burn-up as high as 20atom% has been achieved [13].

5.3. Types of cycles

5.4. Closed cycles

6. Thorium fuel cycle

7. Present and future of Thorium

A. First

Bibliography

[1] K. Kornecki and C. F. Wise, "The role of advanced nuclear reactors and fuel cycles in a future energy system," *PNAS Nexus*, vol. 3, no. 2, 2024. DOI: 10.1093/pnasnexus/pgae030.

[2] J. R. Lamarsh and A. J. Baratta, *Introduction to nuclear engineering*. Prentice Hall; Pearson Education distributor, 2009.

[3] T. J. Dolan, *Molten Salt Reactors and Thorium Energy*, 1st ed. Woodhead Publishing, 2017, ISBN: 0081011261; 9780081011263.

[4] W. M. Stacey, *Nuclear reactor physics Weston M. Stacey*. Wiley-VCH-Verl, 2010.

[5] E. E. Lewis, *Fundamentals of Nuclear Reactor Physics*. Elsevier e-books, 2014.

[6] A. Asghari, "The water neutron detector (wand)," 2016. [Online]. Available: https://api.semanticscholar.org/CorpusID:100282839.

[7] M. S. Jean-Louis Basdevant James Rich, *Fundamentals in nuclear physics: from nuclear structure to cosmology*, 1st ed. Springer, 2005, ISBN: 0387016724; 9780387016726.

[8] J. C. Sanabria, "Reactores nucleares - notas de clase," unpublished, 2021.

[9] K. S. Krane, *Introductory Nuclear Physics*, 2nd. John Wiley, 1988, ISBN: 047180553X; 9780471805533.

[10] N. N. D. Center, *National nuclear data center*, Accessed: 2024-08-24, 2024. [Online]. Available: https://www.nndc.bnl.gov/.

[11] I. A. E. Agency, “Thorium fuel cycle — potential benefits and challenges,” International Atomic Energy Agency, Vienna, Austria, Tech. Rep. IAEA-TECDOC-1450, 2005. [Online]. Available: https://www.iaea.org/publications/7196/thorium-fuel-cycle-potential-benefits-and-challenges.

[12] K. U. e. P. Mohanakrishnan (editor) Om Pal Singh (editor), *Physics of Nuclear Reactors*, 1st ed. Academic Press, 2021, ISBN: 012822441X; 9780128224410.

[13] B. S. Tomar, P. R. V. Rao, S. B. Roy, J. P. Panakkal, K. Raj, and A. N. Nandakumar, *Nuclear Fuel Cycle*. Springer, 2023, ISBN: 9819909481, 9789819909483.

[14] U. E. Humphrey and M. U. Khandaker, “Viability of thorium-based nuclear fuel cycle for the next generation nuclear reactor: Issues and prospects,” *Renewable and Sustainable Energy Reviews*, vol. 97, pp. 259–275, 2018, ISSN: 1364-0321. DOI: https://doi.org/10.1016/j.rser.2018.08.019. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S1364032118305951.

[15] E. E. Lewis, *Fundamentals of Nuclear Reactor Physics*. Academic Press, 2008, ISBN: 0123706319; 9780123706317; 9780080560434; 0080560431.

[16] IEA, *Nuclear power in a clean energy system*, 2019. [Online]. Available: https://www.oecd-ilibrary.org/energy/nuclear-power-in-a-clean-energy-system_fc5f4b7e-en.