APRIL 2018 M.Sc. in Physics Engineering WAHEED ABDI SHEEKHOO

UNIVERSITY OF GAZİANTEP
GRADUATE SCHOOL OF
NATURAL & APPLIED SCIENCES

CALCULATION OF CRITICAL MASS FOR FISSION CHAIN REACTION

M. Sc. THESIS
IN
PHYSICS ENGINEERING

BY
WAHEED ABDI SHEEKHOO
APRIL 2018

Calculation of Critical Mass for Fission Chain Reaction

M.Sc. Thesis

in

Physics Engineering

University of Gaziantep

Supervisor

Prof. Dr. Okan ÖZER

By

Waheed Abdi SHEEKHOO

April 2018

REPUBLIC OF TURKEY

UNIVERSITY OF GAZİANTEP

GRADUATE SCHOOL OF NATURAL & APPLIED SCIENCES

DEPARTMENT OF ENGINEERING PHYSICS

Name of the thesis: Calculation of Critical Mass for Fission Chain Reaction

Name of the student: Waheed Abdi SHEEKHOO

Exam date: 20/04/2018

Approval of the Graduate School of Natural and Applied Sciences

Prof. Dr. Ahmet Necmeddin YAZICI

Director

I certify that this thesis satisfies all the requirements as a thesis for the degree of Master of Science.

Prof. Dr. Ramazan KOÇ

Head of Department

This is to certify that we have read this thesis and that in our consensus; it is fully adequate, in scope and quality, as a thesis for the degree of Master of Science.

Prof. Dr. Okan ÖZER

Supervisor

Examining Committee Members:	Signature
Prof. Dr. Okan ÖZER	....
Prof. Dr. Hakan ÖZTÜRK	....
Assoc. Dr. Mustafa YILMAZ	....

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Waheed Abdi SHEEKHOO

ABSTRACT

CALCULATION OF CRITICAL MASS FOR FISSION CHAIN REACTION

SHEEKHOO, Waheed Abdi

M.Sc. in Physics Engineering

Supervisor: Prof. Dr. Okan ÖZER

April 2018

72 pages

Neutrons at certain energies colliding with fissile nuclei may cause them to undergo fission reaction by splitting into fragments at different masses. Since new neutrons are produced at the end of each fission reaction, a certain amount of fissile material in any type of nuclear reactor core is required for a sustainable chain reaction by these neutrons. It is necessary to determine the amount of mass required for a sustainable fission chain reaction since the procedure is completely random for neutrons to strike target nuclei. It is known that the *critical mass* is the smallest amount of fissile material needed for such a sustainable nuclear chain reaction in any system of geometry. It is obvious that the critical mass of a fissionable material depends upon its nuclear properties such as its fission cross-section, density, shape, enrichment, purity, etc. In this study, the solutions of the steady-state one group diffusion equation are firstly analytically obtained and then compared with numerical results of the *Monte Carlo Method* coded to calculate the critical mass for three basic geometries. The *survival fraction* value, f_s (which is also called as the *multiplication factor*, k) is calculated for the criticality condition for these geometries and the results are tabulated for each one. Our numerical calculations by Monte Carlo Method show that the minimum critical mass is obtained in the case of spherical shape of fuel element for which the analytical solutions are also in aggrement.

Keywords: Chain Reaction, Diffusion Equation, Monte Carlo Method, Critical Mass, Critical Size.

ÖZET

FİSYON ZİNCİR REAKSİYONU İÇİN KRİTİK KÜTLE HESABI

SHEEKHOO, Waheed Abdi
Yüksek Lisans, Fizik Mühendisliği Bölümü
Tez Yöneticisi: Prof. Dr. Okan ÖZER

April 2018
72 sayfa

Belirli enerjilerdeki nötronlar bölünebilir çekirdeklerle çarpışarak onların fisyon sonucu farklı kütlelerdeki parçalarına ayrılmalarına sebep olabilirler. Her bir bölünme sonrası yeni nötronlar üretileceğinden, sürdürülebilir zincir reaksiyonun devamı için herhangi tip nükleer reaktörün merkezinde belli miktarda bölünebilir madde bulunması gerekmekdir. Nötronların hedef çekirdeklerle çarpışması olayı tamamen raslantısal bir durum olduğundan sürdürülebilir zincir reaksiyonu için gerekli kütle miktarının hesabının yapılması gerekmektedir. Kritik kütle ifadesine; herhangi bir geometride nükleer zincir reaksiyonunun sürdürülebilirliği için ihtiyaç duyulan bölünebilir maddenin en az miktarına denildiği bilinmektedir. Bölünebilir malzemenin kritik kütle miktarının maddenin reaksiyon tesir kesit alanına, maddenin yoğunluğuna, şekline, saflığına, zenginleştirme oranına vb. bağlı olduğu çok açıktır. Bu sebeple, difüzyon denkleminin çözümleri çok önemlidir. Tek-grup zamandan-bağımsız difüsyon denkleminin çözümleri analitik olarak elde edildikten sonra sonuçlar Monte Carlo Metodu kullanılarak yazılan bilgisayar programının üç temel geometri için yapılan kritik kütle hesabı sayısal sonuçları ile karşılaştıtılmıştır. *Yaşam faktörü,* f_s, (ki *çoğaltım faktörü,* k, de denilen) parametresi kritiklik şartı için bu geometrilerde hesaplanmış ve sonuçlar her bir geometri için Tablo halinde sunulmuştur. Monte Carlo Metodu ile yaptığımız sayısal hesaplamalarımız, analitik sonuçlarla uyumlu olarak, minimum kritik kütle değerine küresel şekle sahip yakıt elemanının sahip olduğu göstermiştir.

Anahtar Kelimeler: Zincir reaksiyon, Difüzyon denklemi, Monte Carlo Metodu, Kritik kütle, Kritik ebat.

Dedication

To my MOTHER and the soul of my father.

To my brothers and sisters, may God bless them.

To my whole family.

ACKNOWLEDGEMENTS

Firstly, I would like to express my sincere gratitude to my advisor and supervisor Prof. Dr. Okan ÖZER for the continuous support of my M.Sc. study and related research, for his patience, motivation, and immense knowledge. His guidance helped me in all the time of research and writing of this thesis. I could not have imagined having a better advisor and mentor for my M.Sc. study. I have been extremely lucky to have a supervisor who cared so much about my work, and who responded to my questions and queries so promptly.

I would also like to thank all the members of staff at Gaziantep University for the kind opportunity to complete my M.Sc. study.

Last but not the least; I would like to thank my family: my MOTHER, my brothers, sisters and whole family on their unlimited support throughout writing this thesis and my life in general.

TABLE OF CONTENTS

Page

LIST OF FIGURES

Page

LIST OF TABLES

Page

LIST OF SYMBOLS

%	Percentage
$\overline{f_s}$	Average Survival Fraction
B_r	Radial Buckling
B_z	Axial Buckling
B_m	Material Buckling
E_{crit}	Critical Energy
E_q	Coulomb Energy
k_∞	Infinite Medium Multiplication Factor
Σ_f	Macroscopic Fission Cross-Section
Σ_a	Macroscopic Absorption Cross-Section
B_g	Geometrical Buckling
S_n	Rate at which Neutrons are Emitted from Sources per cm^3
f_s	Survival Fraction
n_i	Any Integer Number for the General Solution
β^-	Beta Minus
σ_a	Absorption Cross Section
σ_s	Scattering Cross Section
A	Mass Number
Ba	Barium
Br	Bromine
C	Carbon
Cd	Cadmium
Cs	Cesium
D	Diffusion Coefficient
H	Hydrogen
He	Helium
$\vec{J}$	Neutron Current Density Vector
Kr	Krypton

La	Lanthanum
Li	Lithium
M	Mass of the Rectangular (Cylindrical, Spherical) Block
MCM	Monte Carlo Method
MeV	Mega Electron Volt(s)
Mo	Molybdenum
n	Neutron
N	Number of Randomly Generated Neutrons
Nb	Niobium
Ni	Nitrogen
O	Oxygen
PC	Personal Computer
Pu	Plutonium
R	Radius
Rb	Rubidium
S	Ratio of Length (Height) to Thickness (Radius)
Sb	Antimony
Sr	Strontium
Te	Tellurium
Th	Thorium
U	Uranium
Xe	Xenon
Y	Yttrium
Z	Atomic Number
Zr	Zirconium
M_C	Critical Mass
T	Time for each column
f	Fuel Utilization Factor
γ	Gamma Ray
L^2	Diffusion Area
∇^2	Laplacian
F_2	The Second Fragment
F_1	The First Fragment

CHAPTER 1

INTRODUCTION TO THE STUDY

Over the previous few years, the consumption of electrical energy in all over the world has increased rapidly by huge amounts [1]. Since the population is increasing, the usage of energy is also continuing to grow. Therefore, there are many attempts looking for ways to meet such an enormous amount of energy that the world needs. One of these attempts is to obtain energy coming from the nucleus of an atom. It is well known that there is a great amount of energy holding a nucleus together [2]. This energy may be released in order to produce the heat energy from which one can obtain electrical energy using the heat given off during fission as fuel to turn water into steam in a reactor system. In any ordinary heat-to-electric system, the steam is then used to turn the turbine that can drive generators to produce electricity [3], [4]. This energy can be released in two ways: nuclear fission and fusion. In a nuclear fission, neutrons become a valuable tool for accomplishing fission process and we shall choose the neutrons because of easiness of transacting in comparison with the charged particles whereas neutrons are electrically neutral. It can penetrate toward the nucleus without undergoing Coulomb force with protons or electrons and we cannot accelerate neutrons as the charged particles, in contrast, we could prepare beams of neutrons during conducting a variety of nuclear reactions, the usefulness of these neutrons to induce the fission process and to achieve continuity of fission.

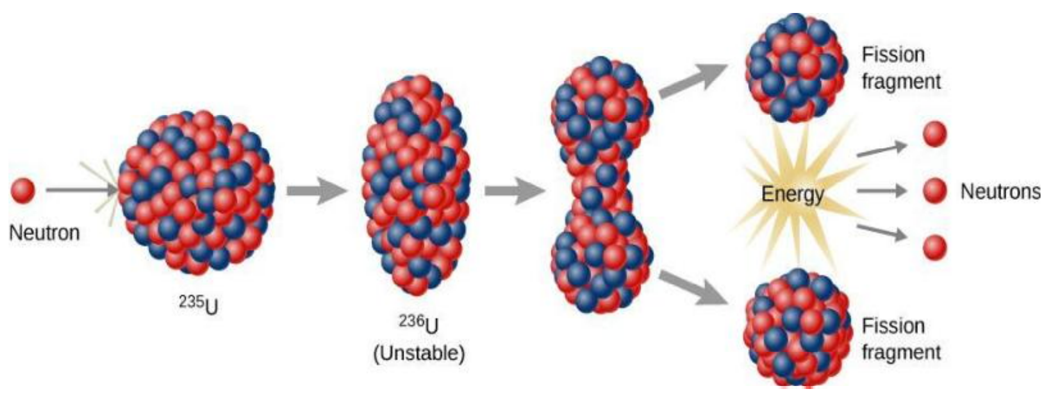


Figure 1.1 Schematic representation of nuclear fission process.

Many extremely important processes occur spontaneously in any nuclear reactor system which is not only the limited to neutron slowdown process as a result of collisions with light or heavy nuclei, but also include the nuclear fission itself and decay of many radioactive nuclei with radiation emissions absorbed through the system or produces decay heat power. To understand how all these physical operations occur in such a system, there is no doubt that having basic information about the nucleus and nuclear reactions with their compositions and the essential forces that have impacted the process is very important [5].

The nucleus consisting of protons and neutrons is the center of the atom. As the number of neutrons is increasing in some very large nuclei, they will be imbalance because of too many neutrons in such isotopes. Therefore, such an imbalance may result in the nucleus becoming unstable. One of the most famous examples is the Uranium-235 isotope which is also a radioactive substance due to its large size can undergo induced fission by thermal neutrons. Thus, it mainly splits into two fragments by giving off energetic neutrons into the medium. There will be two or three neutrons released depending on how the nucleus splits. These new energetic neutrons are decelerated by interactions with the moderator (water, heavy water and graphite) inside the reactor and then they initiate new fission reactions of nuclei of other uranium atoms in the medium. By such a chain reaction more neutrons are released and they cause further nuclear splits. The rate of such a chain reaction can be kept at a constant rate under controlled conditions. This process will produce a heat at high temperatures, but not too much, and can be used to produce electrical energy. If the process is not under control, the reaction can be used as a nuclear bomb. In a nuclear fission chain reaction, neutrons which are emitted during first induced nuclear fission collide with other Uranium-235 nuclei. In such a fission reaction of uranium-235, there is approximately 200 MeV of energy released due to the difference between the sum of the masses of the components and the measured atomic masses in the reaction for reactants and products, respectively [2]. As time goes on, the number of neutrons inside the nuclear system may change such as the rate of production of neutrons, the rate of absorption of neutrons and the rate of leakage of neutrons. Therefore, it is necessary to be a critical reactor through by calculating the critical mass and critical size [4].

Calculation of the critical mass and the critical size of a fuel material in a fission chain reaction are extremely important in nuclear reactor power systems and/or nuclear weapons. There is an exact analogy between the solutions of the one-group steady-state diffusion equation problems with the size and the type of material in the fission process [6]. The fission process not only depends on the neutron energy but it is also related to the type of target material in the reaction. Therefore, the reaction depends on type of neutron interactions, cross sections of target and neutron flux in the system throughout the process. Since the fission is a random process, the simulation of nuclear reaction can be studied by the Monte Carlo Method (MCM) [7]. In random process of fission reactions, one can determine the critical mass and the related critical size of the target material by using a simple computer program via MCM. Using such simple programs one can simulate the solutions of one-group steady state continuity equation for critical size in form of three basic geometries such as rectangular, cylindrical and also in spherical shape.

The purpose of this study is first to review the solution of one-group steady-state diffusion equation for bare systems in three basic geometries, and second to determine the critical mass and the critical size of the hypothetical target material in these geometries for a reactor system, by using MCM. It is considered that such a study will probably help the researchers have an idea about the application of random process by MCM in fission chain reaction and give an idea how to develop the code for further studies in reactor systems.

In their study, Brandon et all [8] determine the critical mass by MCM due to the shape, purity, mean-free path and neutron energy range and report that the lowest critical mass is the spherical one. One may ask here why the lowest critical mass is under investigation: It is obvious that a sustainable chain reaction cannot always result from induced fissions because the notion of "critical mass" which is the *smallest mass* of fissile or other fissionable material in which a self-sustaining chain reaction must occur after induced by neutron. Ibrahim et all [9], [10] also investigate the best description of survival fraction by MCM simulation and report that there are direct connections between the critical mass and parameters such as the dimension of the system and the random points generation for neutrons. There are also some other studies (Gray [11] and Hiroshi et all [12]) for the calculation of critical mass for different types of mixtures with and without a reflector by using some advanced version of MCM packaged programs that use the data library such as JENDL-3.2, ENDF/B-VI and JEF-2.2. All these studies are about the calculation of critical mass but not so simple and easy-to-apply. They need advanced calculations or packaged programs and also some extra data library. In this study our method is very easy, simple and directly applicable even for a hypothetical system. As far as our knowledge, there is no such a simple calculation of critical size and mass of a reactor system by a MCM code that is written and applied in this study.

In Chapter 2, we give general information about the fission reaction, its mechanism, chain reaction, energy range, cross section and neutron flux with their definitions and parameters. In Chapter 3, we review the solution of the one-group steady-state diffusion equation and present the equations for the Buckling parameters to describe the relationship between requirements on fissile material inside a reactor core and dimensions of shape for the core. In Chapter 4, we give briefly the emergence of the MCM and its role to calculate the value of Pi by using random numbers. In Chapter 5, we apply the MCM method to simulate the fission chain reaction in three different geometries. We write a computer code in Wolfram Mathematica [13] and run it for three different shapes of the fuel element. We present our results in Tables and in Figures for each geometry and it is clearly seen that our results are exactly in agreement with those of Diffusion Theory. In Chapter 6, a conclusion is presented.

CHAPTER 2

FISSION CHAIN REACTION

2.1 Fission Mechanism

The fission of Uranium-235 isotope is such a reaction from which one obtains approximately 200 MeV of energy, two lighter nuclei (which are called fission fragments), two or three neutrons, a number of gamma rays and neutrinos [6]. Figure 2.1 shows such a reaction as an example. Since the fission fragments undergo radioactive decay processes, it is not only the energy produced from fission but there are also contributions by neutrons generated in fission and the fission products in each reaction have critical role in nuclear power reactors. On the other hand, we will focus on calculation of the number of neutrons and their distribution in the system.

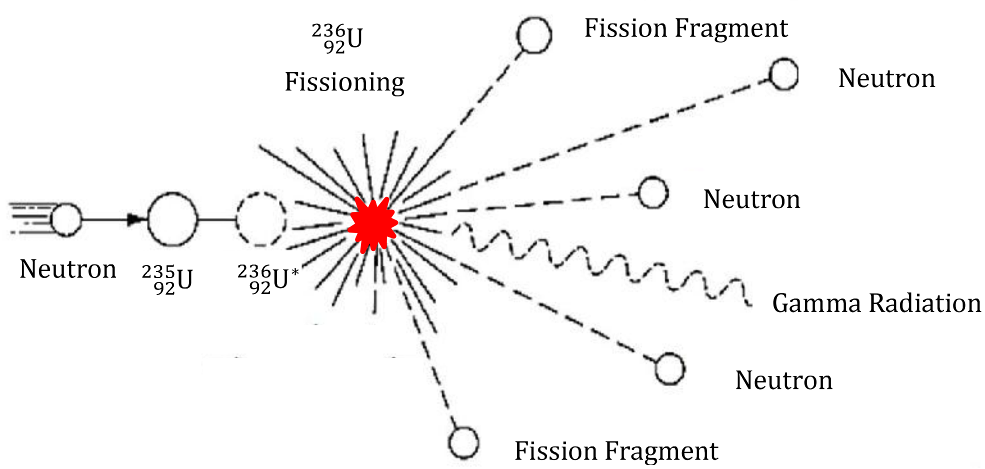


Figure 2.1 Fission Reaction.

The fission fragments are highly excited elements and get rid of this excitation energy by emitting neutrons and also gamma rays. Most of neutrons called as the prompt neutrons are emitted almost immediately ($\sim 10^{-17}\ s$) after the fission takes place and there are some gamma rays known as prompt gammas [14]. Following de-excitation, most of nuclei formed by fission process do not have sufficient excitation energy to emit any more neutrons. They usually decay by beta emission as shown in

Figure 2.2 which is an example decay chain for beta emission. In a few cases, the daughter nuclei created by beta decay may have sufficient energy to emit one neutron. This process has approximately chance of 0.5% or less, and the fission neutrons are observed long after the fission event. These neutrons are called as the delayed fission neutrons.

$$^{139}_{54}Xe \xrightarrow[\gamma]{\beta^-} {}^{139}_{55}Cs \xrightarrow[\gamma]{\beta^-} {}^{139}_{56}Ba \xrightarrow[\gamma]{\beta^-} {}^{139}_{57}La$$

$$n + {}^{235}_{92}\mathrm{U} \longrightarrow n + n + \gamma \text{ (from precursors of Xe} - 139 \text{ and/or Sr} - 95)$$

$$^{95}_{38}Sr \xrightarrow[\gamma]{\beta^-} {}^{95}_{39}Y \xrightarrow[\gamma]{\beta^-} {}^{95}_{40}Zr \xrightarrow[\gamma]{\beta^-} {}^{95}_{41}Nb \xrightarrow[\gamma]{\beta^-} {}^{95}_{42}Mo$$

Figure 2.2 Fission product decay chains for beta decay.

The binding energy per nucleon in a nucleus decreases with increasing mass number for A which is greater than about 50 as shown in Figure 2.3.

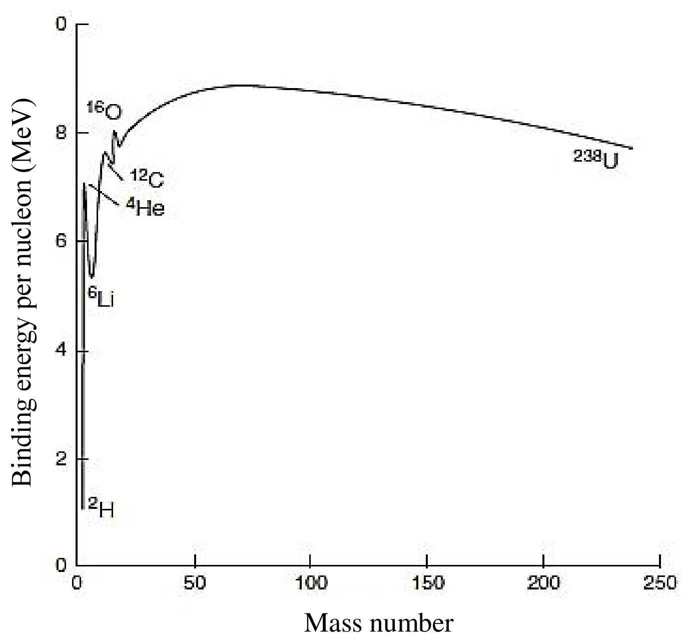


Figure 2.3 Curve of binding energy per nucleon.

In any fission process, it is possible to observe that a heavy nucleus can split into two lighter nuclei which may present relatively more stable configurations. On the other hand, it can also be expected in such nuclear reaction that all heavy nuclei would spontaneously follow fission process, but, it could not exist at all. For a fission process to be taken place with a reasonable probability, some extra energy is to be supplied to the nucleus somehow [6].

The stages of fission process can be given as followings [15]: The initial state of any fissionable nucleus ^{A}Z can be assumed for simplicity to be a spherical shape of radius R as shown in Figure 2.4a. After the fission process, we have two nuclei $^{A}Z_1$ and $^{A}Z_2$ formed by radii R_1 and R_2, respectively, as shown in Figure 2.4c. The details of how the nucleus is actually transformed from the initial (a) to final state (c) are not entirely understood. However, it is assumed that the process involves some sequence of dumbbell-shaped intermediate state shown as in Figure 2.4b.

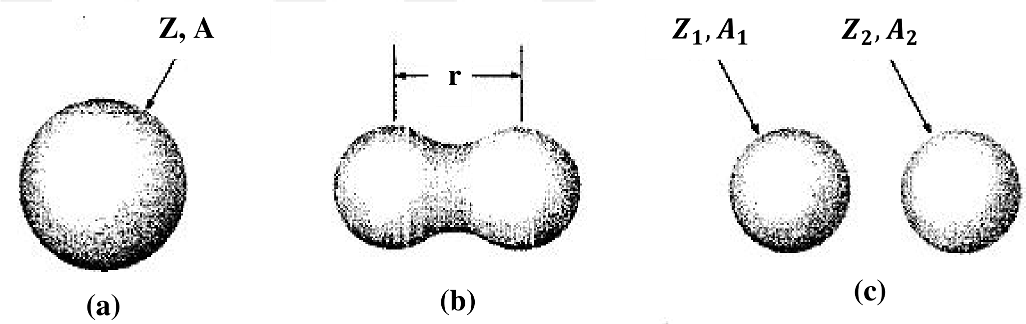


Figure 2.4 Stages in fission.

The potential energy of a fissile nucleus can be given as a function of r between the two separating spheres. The energy is equal to the difference between the total energy of the system at any point and the kinetic energy. If $r = 0$, the total energy of initial nucleus is $M_A c^2$ where M_A is the mass of the initial one for which the total kinetic energy is just zero. To deform this nucleus into a dumbbell-shaped configuration, a certain amount of energy must be added to such system. Since nucleons attract each other, energy is needed to increase the average distance among them. In such an intermediate state the nucleus will have a larger potential energy than it initially had. The potential energy will continue to be increased by increasing r, see Figure 2.5. At a point where two spheres of the dumbbell-shape begin to separate, a certain amount of energy is reached called as the threshold energy or the critical energy (E_{crit}) of the system. After that point, the nuclear energy of two fragments will remain fixed as the potential energy gradually decreases because the Coulomb repulsive energy between two fragments decreases.

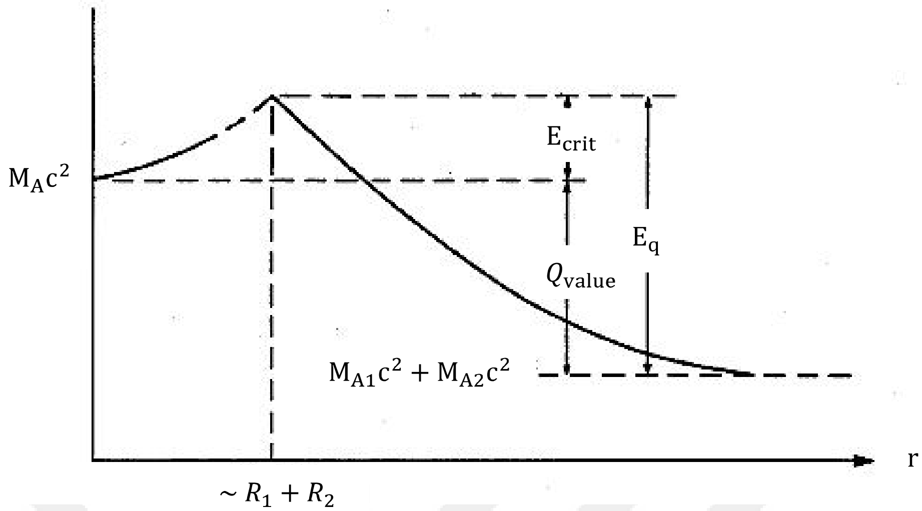


Figure 2.5 Potential energy of nucleus in fission as a function of the distance between the fragmental spheres.

Since the difference between the initial and final energy of the system is called as the $Q-$value of the reaction, E_{crit} is then given simply by the difference between the Coulomb energy E_q at point where fragments starts to separate and the $Q-$value:

$$E_{crit} = E_q - Q_{value} \tag{2.1}$$

Since the masses of all fragments in the fission are not well defined as the initial one, then the $Q-$value for each fission leading to one set of fission fragments is found to be therefore somewhat different from that for fission leading to another. Because of this reason one can say there is no single $Q-$value for all fissions. Thus, the fission $Q-$value may actually be called as the average of the $Q-$value, for all modes of fission reactions. Such a fission $Q-$value is therefore determined experimentally by observing the total energy released in the fission reaction by a mass of nuclei.

If one considers a fission reaction of uranium-235 by a thermal neutron,

$${}^{235}_{92}U + n \longrightarrow {}^{134}Xe + {}^{100}Sr + 2{}^{1}_{0}n + \text{Energy}$$

then one would say that the products are only one set of many possible product nuclei that could be formed by the fission of ${}^{235}_{92}U$. In a fission reaction, there is only one condition to be satisfied is the total number of nucleons in the resultant nuclei must be equal to that of fissionable nucleus and the incident particle inducing the fission. As an example for such a reaction [16], there are 10 possible nuclear fission reactions are given in Table 2.1 as a typical set for fission of uranium-235, and the energy distribution of products in such a process is also given in Table 2.2.

Table 2.1 Set of 10 possible processes (among many other possible reactions) in the fission of $^{235}_{92}U$ with Coulomb repulsion and energy released.

General equation	$^{A}_{Z}U + ^{1}_{0}n \longrightarrow F_1 + F_2 + N\ ^{1}_{0}n + Energy$	Coulomb repulsion (MeV)	Energy released (MeV)
1	$^{235}_{92}U + n \longrightarrow {}^{134}Xe + {}^{100}Sr + 2^{1}_{0}n + Energy$	201.86	180.80
2	$^{235}_{92}U + n \longrightarrow {}^{89}Zr + {}^{144}Ba + 3^{1}_{0}n + Energy$	221.54	181.42
3	$^{235}_{92}U + n \longrightarrow {}^{96}Zr + {}^{136}Xe + 4^{1}_{0}n + Energy$	213.85	188.58
4	$^{235}_{92}U + n \longrightarrow {}^{99}Nb + {}^{133}Sb + 4^{1}_{0}n + Energy$	206.29	177.96
5	$^{235}_{92}U + n \longrightarrow {}^{145}La + {}^{88}Br + 3^{1}_{0}n + Energy$	197.41	168.33
6	$^{235}_{92}U + n \longrightarrow {}^{95}Mo + {}^{139}La + 2^{1}_{0}n + Energy$	235.88	207.78
7	$^{235}_{92}U + n \longrightarrow {}^{144}Ba + {}^{90}Kr + 2^{1}_{0}n + Energy$	199.05	179.57
8	$^{235}_{92}U + n \longrightarrow {}^{141}Ba + {}^{92}Kr + 3^{1}_{0}n + Energy$	199.12	173.28
9	$^{235}_{92}U + n \longrightarrow {}^{94}Zr + {}^{139}Te + 3^{1}_{0}n + Energy$	205.28	172.25
10	$^{235}_{92}U + n \longrightarrow {}^{144}Cs + {}^{90}Rb + 2^{1}_{0}n + Energy$	200.92	175.48
Total		2081.2	1805.41
Average		208.12	180.54

As it is seen, the average energy released in these reactions is 180.54 MeV. There are others energy releases which called delay energy in fission appear as follows:

Table 2.2 The average emitted and recoverable energy values in ordinary thermal neutron induced uranium-235 fission reaction.

Energy type	Source	Average energy released (MeV)
Prompt	kinetic energy of the fission fragments	~168
	kinetic energy of prompt fission neutrons	5
	fission $\gamma -$ rays	7
	$\gamma -$ rays from neutron capture	- (3-9)
Delayed	fission product $\beta -$ decay energy	9 (8)
	fission product $\gamma -$ decay energy	8 (7)
	neutrino kinetic energy	10 (0)
Total fission energy		~207
Recoverable fission energy		198-204

For mechanisms in which some energy is not recoverable in a reactor core is shown in parentheses [16].

For simplicity[17], i.e., $A_1 = A_2 = A/2$ and $Z_1 = Z_2 = Z/2$, may substitute into the equation $E_q = 0.96(Z_1 Z_2/A_1^{1/3} + A_2^{1/3})$ MeV, so the Coulomb repulsion energy[1] give approximately ≈ 206 MeV, the average Q − value energy is ≈ 200 MeV, and therefore the critical energy is found to be about 6 MeV. It is clear that the critical energy value is considerably higher for nuclei lighter than uranium; for example, $E_{crit} \approx 20$ MeV for ^{208}Pb. Because of this, the fission has practical importance only for the heavy nuclei. We present in Table 2.3 the critical energy values of some heavy nuclei which may be called as transuranium elements.

The energy E_{crit} gives us a real threshold energy value for a fission for which any method supplying such energy is called as the "induced fission". The most important method is known as the neutron absorption: The resultant nucleus is formed at such excitation energy which is the summation of the kinetic energy of incident neutron and its binding energy to the final system when a neutron is absorbed. When the binding energy is greater than the critical energy of the compound system, then the fission can take place with induced neutrons having almost zero kinetic energy. For example in Table 2.3 while the critical energy is merely 5.3 MeV for ^{236}U the binding energy is just 6.4 MeV for the last neutron.

Table 2.3 Critical energies and binding energy[2] for fission of different elements.

Fissioning nucleus ^AZ	Critical energy (MeV)	Binding energy of last neutron in ^AZ (MeV)
^{232}Th	5.9	*
^{233}Th	6.5	5.1
^{233}U	5.5	*
^{234}U	4.6	6.6
^{235}U	≈ 6	*
^{236}U	5.3	6.4
^{238}U	5.85	*
^{239}U	5.5	4.9
^{239}Pu	5.5	*
^{240}Pu	4.0	6.4

[1] The Coulomb energy estimates are presumably high because the fragments are surely not spherical at the moment of separation. Also, breakup into equal fragments does not necessarily give the largest energy release, but for the rather crude estimates given here, this is not important.

[2] Neutron binding energies shown by "*" are not relevant for these nuclei since they cannot be formed by the absorption of neutron by the nuclei Z^{A-1}.

When a neutron even at zero kinetic energy is absorbed by ^{235}U nucleus, ^{236}U nucleus is intermediate compound produced at about 1.1 MeV above the critical energy, and then the fission process may immediately take place. Nuclei such as ^{235}U which lead to fission process by following the absorption of a neutron at zero energy are called as “fissile”.

It is also known that the fission reaction can also be induced by process known as photo-fission in which energetic $\gamma-$ rays having greater energy than the critical one. In the design of most nuclear reactors, the photo-fission is usually ignored although there are comparatively some $\gamma-$ rays at such high energies.

In addition to the energy range for fission reaction to occur, any neutron must move through the medium by making collisions even it has high energy. The average distance that a neutron can move through the medium by these collisions is called the *mean free path* shown by “λ”. This quantity can be called as the average value of the distance traversed by a single neutron without a collision in medium.

The value of λ can be obtained from the probability function of p(x) by determining the average distance traveled by neutron:

$$\begin{aligned} \lambda &= \int_0^\infty x\, p(x) dx \\ \lambda &= \Sigma_t \int_0^\infty x\, e^{-\Sigma_t x} dx \\ \lambda &= 1/\Sigma_t \end{aligned} \tag{2.2}$$

It is clearly understandable from the discussion given above that a single nuclear fission of a fissile element produces a great amount of energy. Not only such a huge amount of energy but also the fission makes it attractive that a possible source of commercial power is neutrons which are produced throughout the process itself. If one considers ^{235}U element as fuel, there are averagely of 2.5 neutrons produced per nuclear fission of the element. Because these neutrons can also induce other fissile elements, they may possibly sustain a continuous process in reactor system, and then provide a useful output of energy.

If one defines the ratio of neutrons produced in one generation to that of produced in preceding generation as

$$f_s(\mathrm{k}) = \frac{\text{number of neutrons in one generation } (\mathrm{n_{new}})}{\text{number of fission neutron in the preceding generation } (\mathrm{n_{old}})} \tag{2.3}$$

then one can classify the type of fission chain reaction: If $f_s < 1$ is then the average number of neutrons inducing fission in volume is decreasing, then it is called as “subcritical reactor”. In this case, there is no doubt that the fission process of sample material could not continue indefinitely, and finally the reaction would stop. Therefore, this condition is not desired and not very useful for generating power. If $f_s = 1$, the average number of neutrons inducing fission in volume remains constant throughout the whole process, then it is called as “critical reactor”. In this case, a continued reaction rate in volume is possible. Thus, it is the most expected condition for providing a constant power supply in any nuclear reactor system. If $f_s > 1$, it means that more and more neutrons are produced in volume of fission that results in a runaway chain reaction process. It is called as “supercritical reactor” and it makes the output power grow much more rapidly, than it is desired, leading to an uncontrollable explosion of system [4]–[6]. It is obvious that such kind of process can find its application in a design of nuclear weapon for destructive purposes.

Since neutrons play a key role in the nuclear reactor systems, the neutron flux which means the certain number of neutrons per unit area per unit time must be known. Therefore, neutron flux near the core of any fission reactor is quite high-typically $10^{14}\ neutrons/cm^2 - s$. The energy spectrum of them can extend to 5 to 7 MeV, but generally their peaks are at 1 MeV or at 2 MeV. These high energy neutrons are generally reduced to thermal energies because of collisions within the reactor, but there are possibly some fast neutrons presenting in the core. If a small hole is cut in the shielding barrier of the reactor vessel, a beam of neutrons is possible to be extracted into the laboratory for some experiments. The high energetic neutron’s flux is particularly useful for the production of radioisotopes by neutron capture processes as being done in neutron activation analysis.

The neutrons can be classified according to their kinetic energy as following:

- Thermal neutron E ~ 0.025 eV

- Epithermal neutron $E \sim 1$ eV
- Slow neutron $E \sim 1$ KeV
- Fast neutron $E \sim 1$ KeV $-$ 10 MeV.

2.2 Neutron Interactions with Nuclei of the Absorber

Since neutrons passing through a medium can make different reactions or they just pass through the medium without any interaction with matter, the number and energy range of neutrons change in system. Neutrons are electrically neutral particles and they only make weak interaction with electrons of atoms in which the nucleus is just a positive charge because of protons, and therefore neutrons are not affected by the attractive/repulsive Coulomb force while passing through them. Neutrons may undergo different interactions with nuclei as summarized in the followings [4]–[6]:

2.2.1 Elastic Scattering

In elastic scattering the kinetic energy and momentum are conserved. A neutron colliding with a mass of nucleus M which recoils with an angle φ with respect to the neutron's initial direction of motion is scattered by the nucleus. This is simply the elastic scattering of billiard balls in mechanical physics. If a neutron of mass m_n at initial kinetic energy E_{Ki} is scattered elastically by the nucleus then the kinetic energy transferred to the nucleus can be written generally by

$$\Delta E_K = E_{Ki} \frac{4\, m_n\, M}{(m_n + M)^2} \cos^2\varphi \tag{2.4}$$

It is seen that the possible maximum energy transfer $(\Delta E_K)_{max}$ occurs in head-on collision of particles at which $\varphi = 180^{\circ}$. Then one writes

$$(\Delta E_K)_{max} = E_{Ki} \frac{4\, m_n\, M}{(m_n + M)^2} \tag{2.5}$$

One can also write the average kinetic energy $\overline{\Delta E}_K$ that is gained by the recoil nucleus as

$$\overline{\Delta E}_K = \frac{1}{2} E_{Ki} \frac{4\, m_n\, M}{(m_n + M)^2} = 2\, E_{Ki} \frac{m_n\, M}{(m_n + M)^2} \tag{2.6}$$

The final kinetic energy of neutron E_{Kf} in a head-on collision is equal to

$$E_{Kf} = E_{Ki} - (\Delta E_K)_{max} = E_{Ki}\left(\frac{m_n - M}{m_n + M}\right)^2 \quad (2.7)$$

Since the average energy gained by neutron after scattering is $\overline{E}_{Kf}$, then we have

$$\overline{E}_{Kf} = E_{Ki} - \overline{\Delta E}_K = E_{Ki}\frac{m_n^2 + M^2}{(m_n + M)^2} \quad (2.8)$$

It is seen clearly that the mass of the target element has importance in the elastic scattering: If the target element is hydrogen having nucleus of a proton with mass m_p, then $M = m_p \approx m_n$ and the neutron will directly transfer one half of its initial kinetic energy to the proton. Then the recoil proton may move through a short distance in the absorbing medium and then it may rapidly lose its kinetic energy in the medium because of Coulomb interactions with other nuclei and/or orbital electrons of the medium.

2.2.2 Inelastic Scattering

In such interactions, a neutron is captured and re-emitted with a lower energy by a nucleus in any direction different from absorbed neutrons'. After the interaction, nucleus is now in its excited state and will become stable by emitting gamma rays with high energy. This process can be illustrated by the following reaction:

$$n + {}^{A}_{Z}X \longrightarrow {}^{A+1}_{Z}Y^* \longrightarrow {}^{A}_{Z}X^* + n \Longrightarrow {}^{A}_{Z}X^* \longrightarrow {}^{A}_{Z}X + \gamma$$

where

${}^{A}_{Z}X$ is the target nucleus.

${}^{A+1}_{Z}Y^*$ is an unstable compound nucleus.

${}^{A}_{Z}X^*$ is an excited target nucleus.

2.2.3 Neutron Capture

It is a kind of reaction in which a thermal neutron getting reaction with a nucleus leads to the emission of gamma ray or a proton if possible. Two of them have particular importance: ${}^{14}Ni(n,p){}^{14}C$ and ${}^{1}H(n,\gamma){}^{2}H$ and the other one ${}^{113}Cd(n,\gamma) - {}^{114}Cd$, is also important in process of shielding against thermal neutrons that may lead the system "supercritical".

2.2.4 Spallation

It occurs if a fast neutron penetrates through the nucleus and gives sufficient amount of energy to the nucleus. Then the nucleus may disintegrate into residual particles such as $\alpha -$ particles, protons and neutrons. The following process is an example:

$$^{16}_{8}O + n \longrightarrow 3\alpha + 2p + 3n$$

Most of the energy released in such process is carried away from the system by heavier fragments that may leave their energy in the absorber in the medium. However, neutrons and gamma rays carry their energy to further location.

2.2.5 Fission Induced by Neutron

Fission is a special type of neutron interaction in which thermal neutrons bombard certain amount of very heavy nuclei [14]. The products are nuclei of lower atomic number and generally there are fast neutrons more than one as output. Materials undergoing the fission reaction by *thermal neutrons* are called fissile or fissionable materials. The most famous fissionable materials are known as:

- U-235 (0.7% of naturally occurring uranium)
- Pu-239 produced from uranium-238
- U-233 produced from thorium-232

It is necessary to note here that U-233, U-235 and Pu-239 which undergo fission reaction rapidly by thermal neutron capture are important for nuclear reactors [18]. On the other hand, U-238 and Th-232 are called fertile nuclides which undergo fission themselves but transform into fissionable nuclides if they are bombarded with neutrons. After the fission process of a fissionable nucleus, lighter and generally radioactive products called as fission fragments are produced. These fragments are called as fission products and they have great importance in the calculation of Decay-Heat-Power in any reactor after the shot-down process or in a nuclear reactor accident.

2.3 Cross Section

The mass, charge and energy of incident particle determines the interaction of probability with the target element which is assumed to be at rest. The target nuclei also have these parameters; they will also affect the probability calculation of any interaction in the process. All these effects for the target nucleus are totally given by the term “cross-section” for the interaction. It is shown by σ_i where i defines the type of the interaction.

In a nuclear fission, the parameter cross-section σ has the meaning of the probability of a certain nuclear reaction occurring and is defined as a surface value. It is the probability that a particle will interact per unit surface area of target, and this area defines the unit for cross-section in barn, b, which is generally used to describe the probability of reaction in atomic and nuclear physics. It is defined as $1b=10^{-24}cm^2$.

2.4 Neutron Flux

Suppose that a beam of mono-energetic neutrons “n” number of neutrons per cm^3 with average velocity v in a beam are incident on a thin-target of thickness X and having area of A, then the intensity neutron beam is defined as

$$I = nv \tag{2.9}$$

Since the neutrons move the distance v cm in 1 sec, all neutrons in the volume vA in front of the target will strike it in 1 sec. Thus, one can write $nvA = IA$ neutrons strike the entire target per second, and it follows that $IA/A = I$ is equal to the number of neutrons striking the target per $cm^2\ /sec$. Since nuclei are small and the target is assumed to be thin, most of the neutrons striking the target in an experiment like that shown in Fig. 2.6 ordinarily pass through the target without interacting with any of the nuclei. The numbers that do collide are found to be proportional to the beam intensity, to the atom density N_a of the target, and to the area and thickness of the target. These observations can be summarized by the equation:

$$Number\ of\ collisions\ per\ second\ (in\ entire\ target) = \sigma\ IN_aAX \tag{2.10}$$

where σ is called the cross-section. The factor N_aAX is the total number of nuclei in the target.

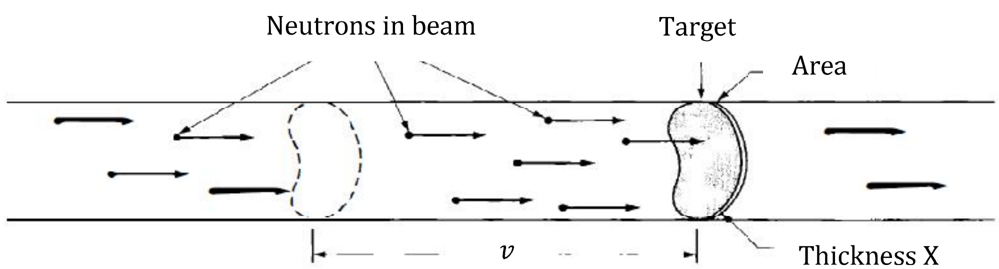


Figure 2.6 Neurton beam striking a tirget.

Neutron beam is assumed to strike all the target. Since the neutron beam has much smaller area than the target, one can consider "neutron strike area" instead of "whole area" for the term "A". In all processes characteristic cross-section of nucleus that interacts with neutron is defined. The total cross-section, σ_t, is given as the sum of the scattering and the absorption cross-section of the target as

$$\sigma_t = \sigma_s + \sigma_a$$

Thus, it gives the probability of any type of reaction may ocur in the system.

If one writes the latest equation again

$$\text{Number of collisions per second (in entire target)}\ IN_a\sigma_t \times \mathrm{AX} \quad (2.11)$$

where "AX" is the total volume of the target element for the number of collisions per $cm^3\ /sec$. Therefore, one can define the collision density, F, given by

$$F = IN_a\sigma_t \quad (2.12)$$

in which one can also define the macroscopic cross-section, $\sum_\mathrm{t}$, that has great importance in in nuclear engineering as

$$\mathrm{F} = I\sum\nolimits_\mathrm{t} \quad (2.13)$$

In an hypothetical experiment as given in Figure 2.7, neutron beams at different intensities with the same energies may incident on the target material. Then one can write the total interaction rate as

$$F = \sum\nolimits_t (I_A + I_B + I_C + \cdots) \quad (2.14)$$

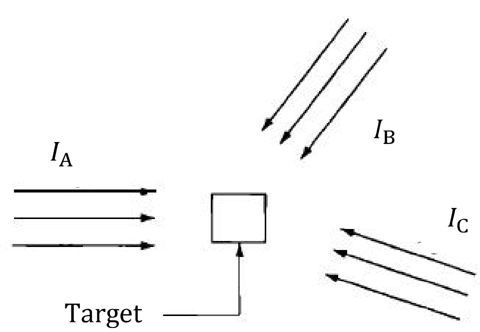


Figure 2.7 Neurton beams striking a tirget.

Since the intensity is defined as $I = nv$, then Eq. (2.14) is written as

$$F = \sum_t (n_A + n_B + n_C + \cdots)v \qquad (2.15)$$

where $(n_A + n_B + n_C + \cdots)$ is defined as the total density of neutrons beams and v is the average neutron speed. Then one gets

$$F = \sum_t nv \qquad (2.16)$$

The quantity "nv" is now called as the *neutron flux* in the system and shown by the symbol ϕ:

$$\phi = nv \qquad (2.17)$$

The colission density is now given as

$$F = \sum_t \phi \qquad (2.18)$$

Since the neutron beam consists of neutrons at different energies, then the energy distribution of neutrons can be defined as $n(E)$. Then the neutron density per unit energy $n(E)d(E)$ is given for the number of neutrons per cm^3 that energies between E and $E + dE$. Then, one writes the collision density rate as

$$dF = \sum_t (E) \times n(E)dE \times v(E) \qquad (2.19)$$

in which all parameters are energy dependent. The total reaction density is now given by

$$F = \int_0^\infty \sum_t(E)n(E)v(E)\,dE = \int_0^\infty \sum_t (E)\phi(E)dE \qquad (2.20)$$

where $\phi(E) = n(E)v(E)$ is called the flux per unit energy.

It is clear that Eq. (2.20) is written for the total interaction rate. For particular type of interactions, it can be written by similar expressions such as

$$F_s = \int_0^\infty \sum_s (E)\phi(E)dE \quad and \quad F_a = \int_0^\infty \sum_a (E)\phi(E)dE \qquad (2.21)$$

for the number of scattering collision rate and that of the absorption rate in the system and so on.

CHAPTER 3

DIFFUSION THEORY

3.1 Introduction

Diffusion theory provides quite applicable mathematical description of the neutron flux in non-multiplicative and multiplicative reactor medium when some assumptions made in its derivation are satisfied for conditions such as absorption much less likely than scattering, linear spatial variation of the neutron distribution, isotropic scattering etc. [7], [19]–[21]. These are given as followings: The first condition can be satisfied by most of the moderating (such as water, graphite) and structural materials found in reactor system, but not by the fuel itself and control elements. The second condition can be available for a few mean free paths that are away from the boundary of large homogeneous media due to a relatively uniform source distributions. The third condition can be valid for neutrons scattering from nuclei having heavy atomic mass. Since a reactor system consists of many thousands of elements, such as highly absorbing materials with different dimensions on the order of different mean free paths or less, diffusion theory can be widely applicable and used in analysis of nuclear reactor problems and it gives quite accurate predictions in the solutions of such systems.

3.2 Diffusion Equation for Critical Reactor

Having a self-sustaining chain reaction, the number of neutrons that are emitted through fission processes must be known and the ratio of the total number of neutrons in one generation divided by the total number of fission neutrons in the preceding generation is given by the symbols f_s or k which are generally called as the *survival fraction* or *multiplication factor*, respectively. In a simple equation, it can be given by:

$$f_s\,(\mathrm{k}) = \frac{\text{number of neutrons in one generation } (\mathrm{n_{new}})}{\text{number of fission neutron in the preceding generation } (\mathrm{n_{old}})} \tag{3.1}$$

In order to determine the possibility for a chain reaction to occur, the value of k must be known for fission neutrons which will effectively induce another fission reaction.

If $k > 1$, then the reaction is in the supercritical regime which means that the nuclear material has a mass greater than critical mass required. Then more and more neutrons are produced at every stage of fission, causing a runaway chain reaction and it causes the output energy to grow rapidly, leading to an uncontrollable explosion. Needless to say, this kind of condition finds application in the design of nuclear weapons.

If $k < 1$, then the rate of chain reaction decreases with time and it is called the sub-critical regime where the reactor never achieve a critical state. It is clear that in this case the fissioning of some sample of material cannot continue indefinitely, and eventually the reaction stops. This condition is therefore not very useful for generating power.

If $k = 1$, then it is called the critical regime which is the required state in which the chain reaction occurs at a constant level and therefore the energy released in the reactor volume is at a steady level. Such a system does not depend on time and said to be critical. The number of neutrons inducing fission remains constant at every stage. In this case, a continued reaction rate is possible. This is the most desirable condition for providing a constant supply of power in a nuclear reactor.

For a reactor at critical state, determination and control of the number of neutrons in the volume must be balanced with the production rate of neutrons produced within the reactor and the absorption rate of them in nuclear reactions, plus, the leakage rate of neutrons escaping from the surface of the reactor [22]. Therefore, to have the k-value equal to one the absorption rate of neutrons summed up with escaping rates must be equal to the production rate of neutrons. Thus, one can write

$$k_c = \frac{\text{neutrons productions}}{\text{neutrons absorbtions} + \text{neutrons escaping (leakage)}} = 1 \qquad (3.2)$$

If V is a volume of medium containing neutrons, three options can be given as following: Firstly, neutrons are produced within the volume. Secondly are neutrons absorbed within the volume, and the final one is neutrons are escaping (leakage) from the volume. It is obvious that all these options are possibly changing with time and they go on randomly. Thus, the rate of change of neutrons in such a volume can be given by a simple equality which can be called as the equation of continuity [4], [20], [23]:

$$\begin{aligned} &\text{Rate of change in number of neutrons in V} \\ &\quad = +\text{Neutron production rate in V} \\ &\qquad - \text{Neutron obsorbtion rate in V} \\ &\qquad - \text{Neutron Leakage rate in V} \end{aligned} \tag{3.3}$$

where:

$$\text{Rate of change in number of neutrons in V} = \int_V \frac{\partial n}{\partial t}\, dv$$

$$\text{Neutron production rate in V} = \int_V S_n\, dv$$

$$\text{Neutron obsorbtion rate in V} = \int_V \Sigma_a \phi\, dv$$

For the leakage rate, one has to use the Fick’s law. Fick's law is simply based an idea for any solute diffusing from a greater dense region to a lower dense region in any solution. In the reactor volume, one can assume that the medium is as a solution and the neutrons as solute material.

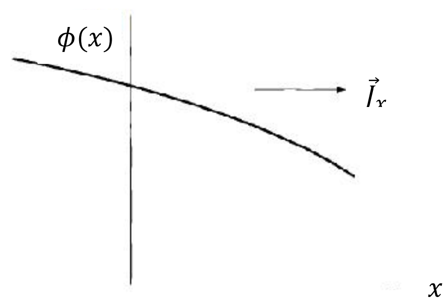


Figure 3.1 Neutron flux and neutron current density vector.

Fick’s law states that the current density vector of the solute in the solution is given by

$$\vec{J} = -D\,\vec{\nabla}\phi$$

where $\vec{J}$ is defined as the net number of neutrons passing through unit area per unit time. It is seen that $\vec{J}$ is a vector quantity with the same unit as flux ($neutrons/cm^2 - sec$). D is called as the Diffusion coefficient in unit of *cm*. $\vec{\nabla}$ is the gradient operator for three spatial variables.

Thus, one can write the neutron leakage rate in volume as

$$\text{Neutron Leakage rate in V} = \int_A \vec{J} \cdot d\vec{A}$$

By using the divergence theorem, one can transform the surface integral into a volume integral as following:

$$\text{Neutron Leakage rate in V} = \int_A \vec{J} \cdot dA = \int_V \operatorname{div} \vec{J}\ dV$$

Rewriting all integral forms in the equation of continuity, one gets

$$\int_V \frac{\partial n}{\partial t}\, dv = \int_v S_n\, dv - \int_v \Sigma_a \phi\, dv - \int_V \operatorname{div} \vec{J}\ dV$$

Since the integrals are for the same volume element, one writes [19]

$$\frac{\partial n}{\partial t} = S_n - \Sigma_a \phi - \operatorname{div} \vec{J} \tag{3.4}$$

The Eq. (3.4) is the *general form of the equation of continuity*. If the system is assumed to be steady-state,

$$S_n - \Sigma_a \phi - \operatorname{div} \vec{J} = 0 \tag{3.5}$$

The Eq. (3.4) is now known as the *steady state equation of continuity*. From the Fick's law, one knows

$$\vec{J} = -D\, \vec{\nabla}\, \phi$$

and

$$\operatorname{div} \vec{J} = -D\, \nabla^2\, \phi$$

where the flux for the one-group energy of neutrons is

$$\phi = nv$$

Thus, one gets from Eq. (3.4)

$$D\, \nabla^2 \phi - \Sigma_a \phi + S_n = 0 \tag{3.6}$$

The Eq. (3.5) is called as the *steady-state diffusion equation*.

Since a measurable power in a reactor volume depends mainly on the source neutrons which are emitted in sustainable fission reaction, the source term S can be defined as

$$S_n = \nu\, \Sigma_f\, \phi$$

where Σ_f is the microscopic fission cross-section for the fuel and ν is the average number of neutrons produced per fission in the reaction. If the fission source could not balance the leakage and absorption terms in Eq. (3.6), then the equation would be nonzero. Having a balance in the equation, one can multiply the source term with a constant $1 / \mathrm{k}$, where k is an unknown constant for now. Therefore, one writes

$$\mathrm{D}\,\nabla^2\phi - \Sigma_a\phi + \frac{1}{\mathrm{k}}\nu\,\Sigma_f\,\phi = 0 \tag{3.7}$$

After rearranging the equation, one obtains

$$B^2 = \frac{1}{D}\left(\frac{1}{\mathrm{k}}\,\Sigma_f - \Sigma_a\right)$$

and then Eq. (3.7) may now be written in the following form:

$$\nabla^2\phi = -\mathrm{B}^2\phi \tag{3.8}$$

where B^2 is defined as the *geometric buckling*.

If Eq. (3.8) is substituted into Eq. (3.7) for $\nabla^2\phi$, one gets

$$-\mathrm{D}\,\mathrm{B}^2\phi - \Sigma_a\phi + \frac{1}{\mathrm{k}}\nu\,\Sigma_f\,\phi = 0 \tag{3.9}$$

Eq. (3.9) is called as the *one group reactor equation*.

In reactor volume the neutrons are not only absorbed by the fuel but they are also absorbed by the environment elements such as moderator. Therefore, the source term in the one group equation should be written in its more general form: If Σ_{aF} is the absorption cross section for the fuel element in one group energy equation and η is the average number of fission neutrons emitted per neutron absorbed by the fuel, one can then write the source term as

$$\mathrm{S}_n = \eta\,\Sigma_{aF}\,\phi \tag{3.10}$$

If one assumes that f is the fraction for number of neutrons absorbed by the fuel element to the total number of neutrons absorbed by the mixture of fuel and moderator in the reactor volume, then one can write

$$f = \frac{\Sigma_{aF}}{\Sigma_a} \tag{3.11}$$

where f is called as the *fuel utilization coefficient* of the system. By using Eq. (3.11) into Eq. (3.10) for the term Σ_{aF} one finds

$$S_n = \eta \, \Sigma_{aF} \frac{\Sigma_a}{\Sigma_a} \, \phi = \eta \, f \, \Sigma_a \, \phi \tag{3.12}$$

Here again, the term Σ_a is the summation of cross sections for the mixture of fuel and moderator elements and Σ_{aF} is only the cross section of the fuel itself. One can write Eq. (3.12) in terms of multiplication factor, k, for an infinite reactor in which there are no neutrons escaped (but absorbed fully) from the surface of reactor system. All neutrons are absorbed either in the fuel or by the coolant eventually. Therefore, the absorption rate of $\Sigma_a \, \phi$ neutrons in one generation will lead to the absorption rate of $\eta f \Sigma_a \, \phi$ neutrons. Since the definition of multiplication factor is the division of total number of fissions in one generation by that of in the preceding generation then one writes

$$k_\infty = \frac{\eta \, f \, \Sigma_a \, \phi}{\Sigma_a \, \phi} = \eta f \tag{3.13}$$

This result is only applicable for an infinite reactor volume. (One can consider the four factor formula: $k_\infty = \varepsilon \, p \, \eta \, f$. It is also completely independent of size and shape of reactor by describing the inherent multiplication ability of fuel and moderator without regard to leakage.) Then the source terms in Eq. (3.12) can now be written as

$$S_n = k_\infty \, \Sigma_a \, \phi \tag{3.14}$$

Replacing Eq.(3.14) and Eq.(3.8) into Eq.(3.7) one gets

$$- D \, B^2 \phi - \Sigma_a \phi + \frac{k_\infty}{k} \Sigma_a \phi = 0 \tag{3.15}$$

If the reactor system is in critical condition, then one sets k=1. If one defines the parameter, called as *diffusion area*, by

$$L^2 = \frac{D}{\Sigma_a}$$

then Eq.(3.15) can now be written as

$$- B^2 \phi + \left(\frac{k_\infty - 1}{L^2} \right) \phi = 0 \tag{3.16}$$

in which one deals with the material properties of the reactor system such as the type of fuel, type of moderator etc. Thus, Eq.(3.16) gives a new definition of the buckling parameter for a critical reactor as

$$\mathrm{B}^2 = \frac{\mathrm{k}_\infty - 1}{\mathrm{L}^2} = \mathrm{B}_g^2 = \mathrm{B}_m^2 \tag{3.17}$$

where B_g is called as the geometrical buckling and B_m is the material buckling.

3.3 Calculation of Geometric Buckling for Some Reactor Shapes

In this section, we briefly present the derivation of geometric buckling parameter for three different geometries.

3.3.1 Spherical Reactor

A bare spherical reactor of radius R is considered. The Laplacian operator is

$$\nabla^2 = \frac{1}{\mathrm{r}^2}\frac{d}{dr}\left(\mathrm{r}^2\frac{d}{dr}\right) \tag{3.18}$$

Using Eq. (3.18) into Eq. (3.8), one gets

$$\frac{1}{\mathrm{r}^2}\frac{d}{dr}\left(\mathrm{r}^2\frac{d\phi}{dr}\right) + \mathrm{B}^2\phi = 0 \tag{3.19}$$

For the solution of Eq. (3.19) one can define

$$\phi = \omega/r \tag{3.20}$$

By the substitution of Eq. (3.20) into Eq. (3.19), one obtains

$$\frac{1}{\mathrm{r}^2}\frac{d}{dr}\left(\mathrm{r}^2\frac{d}{dr}\frac{\omega}{r}\right) + \mathrm{B}^2\frac{\omega}{r} = 0 \tag{3.21}$$

After some algebra, one finally finds

$$\frac{d^2\omega}{dr^2} + \mathrm{B}^2\omega = 0 \tag{3.22}$$

The general solution of the Eq. (3.22) is found to be as

$$\omega = A\sin(B\,r) + C\cos(B\,r) \tag{3.23}$$

where $\omega = r\,\phi$. Then Eq. (3.23) may be written as

$$\phi(\mathrm{r}) = \mathrm{A}\,\frac{\sin(B\,r)}{r} + \mathrm{C}\,\frac{\cos(B\,r)}{r}$$

in which A and C are constants. Using the boundary conditions one can conclude that if *r* goes to zero, the term "cos(B *r*) / *r*" goes to infinity. Since the flux is a physical quantity for neutrons in the system, this result is physically not acceptable. Therefore, C=0. The final solution of the flux equation for the spherical reactor is found to be

$$\phi = \mathrm{A}\,\frac{\sin(B\,r)}{r} \tag{3.24}$$

For the second boundary condition: $\phi(\mathrm{R}) = 0$, it can be satisfied (by the Zero Flux Boundary method as discussed in Ref. [20], [23]) by setting B as

$$B_n = \frac{n_i\,\pi}{R}$$

where n_i is any integer number for the general solution. However, we set n_i=1 because we deal with the neutron flux equation which is solved for "particles" but not for "waves". Thus, the geometric buckling for a critical sphere of radius is found to be

$$\mathrm{B}^2 = \left(\frac{\pi}{R}\right)^2 \tag{3.25}$$

The calculation of the constant A in the flux equation is related with the power of the reactor and the reactor volume.

3.3.2 Rectangular Reactor

In this geometry, the flux depends on the spatial axes and one can use the Cartesian Coordinate System for the solution of Eq.(3.8). We consider a rectangular parallelepiped shape of side lengths "a, b and c". The origin of the coordinate system is assumed to be located at the center of the shape. Then the reactor equation becomes

$$\frac{\mathrm{d}^2\phi}{\mathrm{dx}^2} + \frac{\mathrm{d}^2\phi}{\mathrm{dy}} + \frac{\mathrm{d}^2\phi}{\mathrm{dz}^2} + \mathrm{B}^2\phi = 0 \tag{3.26}$$

Using the separation of variables for $\phi = \phi(\mathrm{x,y,z}) = \mathrm{f(x)\,g(y)\,h(z)}$ one writes

$$\frac{1}{\mathrm{f(x)}}\frac{\mathrm{d}^2\mathrm{f(x)}}{\mathrm{dx}^2} + \frac{1}{\mathrm{g(y)}}\frac{\mathrm{d}^2\,\mathrm{g(y)}}{\mathrm{dy}} + \frac{1}{\mathrm{h(z)}}\frac{\mathrm{d}^2\mathrm{h(z)}}{\mathrm{dz}^2} = -\mathrm{B}^2 \tag{3.27}$$

The terms on the left hand side of Eq. (3.27) are functions of x, y, z respectively, and the term on the right hand side is just a constant. Therefore one can get

$$\begin{aligned}\frac{1}{f(x)}\frac{d^2f(x)}{dx^2} &= -B_x^2\\ \frac{1}{g(y)}\frac{d^2\,g(y)}{dy} &= -B_y^2\\ \frac{1}{h(z)}\frac{d^2h(z)}{dz^2} &= -B_z^2\end{aligned} \tag{3.28}$$

where $B_x^2 + B_y^2 + B_z^2 = B^2$. One can now determine the flux function within the reactor volume: Eq. (3.28) must be solved for the subject to the boundary condition that each function must vanish at the faces on each axis: That means, for example, for the x-axis

$$f\left(\frac{a}{2}\right) = f\left(-\frac{a}{2}\right) = 0 \tag{3.29}$$

It must also be noted here that because of the symmetry of the problem, there shall be no net flow of neutrons at the center of the rectangle. Because the neutron current density is directly proportional to the derivative of $f(x)$, then the general solution of the Eq. (3.28) is

$$f(x) = A\cos(B_x\,x) + C\sin(B_x\,x) \tag{3.30}$$

where A and C are constant to be determined. Since there is flux at the center of the system then one sets $C = 0$ to satisfy the boundary condition. Then we have

$$f(x) = A\cos(B_x\,x) \tag{3.31}$$

Introducing the boundary condition for $x = a/2$, we find

$$f(a/2) = A\cos\left(B_x\,\frac{a}{2}\right) = 0 \tag{3.32}$$

which leads to the trivial solution

$$\cos\left(B_x\,\frac{a}{2}\right) = 0 \tag{3.33}$$

Eq. (3.33) should be equal $(n\pi/2)$, where n is an odd integer if the reactor is critical. Since all functions except the first die out for neutron flux, the buckling is to be the first eigenvalue of the solution when $n = 1$.Thus,

$$B_x = \frac{\pi}{a}$$

One can solve the Eq. (3.28) by the same way for the other axis, and in that case, and one obtains finally the solution to be a purely a cosine function for all. Therefore, the flux function is

$$\phi(x, y, z) = f(x)g(y)h(z) = \cos(B_x\, x) \cos(B_y\, y) \cos(B_z\, z) \tag{3.34}$$

in which the total buckling for the rectangular parallelepiped is found as

$$B^2 = B^2(x) + B^2(y) + B^2(y) = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2 \tag{3.35}$$

3.3.3 Infinite - Cylindrical Reactor

The flux is only the function of the distance r from the axis in infinite height of cylindrical reactor of radius R. The reactor equation is written only for the radial component of the Laplacian operator as

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\phi}{dr}\right) + B^2\phi = 0 \tag{3.36}$$

Eq. (3.36) is a special case of Bessel’s equation of the form

$$\frac{d^2\phi}{dr^2} + \frac{1}{r}\frac{d\phi}{dr} + \left(B^2 - \frac{m^2}{r^2}\right)\phi = 0 \tag{3.37}$$

where m is a constant and Eq.(3.37) has two independent solutions called as ordinary Bessel functions of the first and second kind, respectively, denoted as $J_m(Br)$ and $Y_m(Br)$. When comparing Eq. (3.37) with Eq. (3.36) it shows that the parameter m should be equal to zero, and therefore the general solution to the reactor equation is written as

$$\phi(r) = A\, J_0(Br) + C\, Y_0(Br) \tag{3.38}$$

where A and C are again constants. The general form of functions $J_0(Br)$ and $Y_0(Br)$ are plotted in Fig. (3.2). Since $Y_0(x)$ goes to infinity as $x \to 0$, such a physical solution for the neutron flux is not physically acceptable. However, $J_0(0) = 1$ when $x = 0$. Therefore, it satisfies the condition for flux remains finite within the reactor, and then one assumes $C = 0$. The only solution of the flux is

$$\phi(r) = A\, J_0(Br) \tag{3.39}$$

Applying the boundary condition $\phi(R) = 0$ we write

$$\phi(R) = A\, J_0(B\, R) = 0 \tag{3.40}$$

where the function $J_0(x) = 0$ is satisfied for different values of x labeled as $x_1, x_2, ..$ in Fig. (3.2). So, the general function for the condition is given by $J_0(x_n) = 0$.

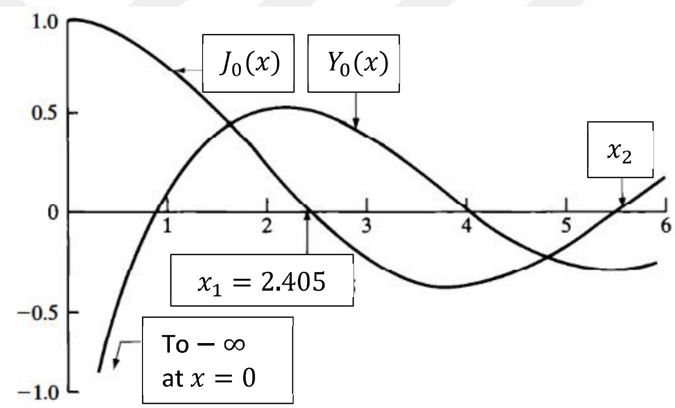


Figure 3.2 The Bessel functions $J_0(Br)$ and $Y_0(Br)$.

Therefore, Eq. (3.40) has solution for B values satisfying the condition

$$B_n = \frac{x_n}{R} \tag{3.41}$$

In a critical reactor for k=1, only the lowest eigenvalue is taken into account and then the geometric buckling is found to be

$$B_1^2 = \left(\frac{2.405}{R}\right)^2 \tag{3.42}$$

3.3.4 Finite - Cylindrical Reactor

In this reactor geometry, the flux does not depend only on the radius of the cylinder but also the distance z (Height) from the midpoint of the cylinder. Using the cylindrical co-ordinate system one can write the reactor equation as

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\phi}{dr}\right)+\frac{d^2\phi}{dz^2}+B^2\phi=0 \tag{3.43}$$

Using the separation of variable method for $\phi(r,z)=R(r)\,Z(z)$ one writes

$$\frac{1}{R}\frac{1}{r}\frac{d}{dr}\left(r\frac{dR}{dr}\right)+\frac{1}{Z}\frac{d^2Z}{dz^2}=B^2 \tag{3.44}$$

and then one gets

$$\begin{gathered}\frac{d^2R}{dr^2}+\frac{1}{r}\frac{dR}{dr}=B_r^2R\\ \frac{d^2Z}{dz^2}=B_z^2Z\end{gathered} \tag{3.45}$$

where the total buckling B^2 is

$$B^2=B_r^2+B_z^2 \tag{3.46}$$

Eq. (3.45) is similar to that of equation for the rectangular reactor and therefore has the similar process for the solutions of equalities in the form. One finds

$$\begin{gathered}B_r^2=\left(\frac{2.405}{R}\right)^2\\ B_z^2=\left(\frac{\pi}{H}\right)^2\end{gathered} \tag{3.47}$$

for each axis. Then the final result for the geometric buckling is given as

$$B^2=\left(\frac{2.405}{R}\right)^2+\left(\frac{\pi}{H}\right)^2 \tag{3.48}$$

3.4 Theoretical Calculation of the Critical Mass

This section includes equations regarding the critical cases of the three geometrical shapes (Rectangular parallelepiped, Cylindrical and Spherical) to be a good platform for the calculation of critical mass via MCM.

3.4.1 For a bare rectangular parallelepiped

In the rectangular parallelepiped, when we change the shape to obtain the minimum mass, there is a special case when the three sides are equal to each other that implies it also inclusive the cubic shape.

Using Eqs.(3.17) and (3.45) together one writes

$$B_m^2 = B_g^2 \Longrightarrow \frac{k_\infty - 1}{L^2} = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2 \tag{3.49}$$

The critical volume and the critical mass for a certain density of material are given by

$$V_C = a \times b \times c \text{ and } M_C = \rho V_C \tag{3.50}$$

3.4.2 For a bare finite cylinder

Using again Eqs.(3.17), (3.46) and (3.47) together one writes

$$B_m^2 = B_g^2 \Longrightarrow \frac{k_\infty - 1}{L^2} = \left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2 \tag{3.51}$$

The critical volume and the critical mass for a certain density of material are given by

$$V_C = \pi R^2 H \text{ and } M_C = \rho V_C \tag{3.52}$$

3.4.3 For a bare sphere

Using Eqs.(3.17) and (3.25) one writes

$$B_m^2 = B_g^2 \Longrightarrow \frac{k_\infty - 1}{L^2} = \left(\frac{\pi}{R}\right)^2 \tag{3.53}$$

and the critical radius is found to be

$$R = \pi \sqrt{\frac{L^2}{k_\infty - 1}} \tag{3.54}$$

The critical volume and the critical mass for a certain density of material are given by

$$V_C = \frac{4}{3} \pi R^3 \text{ and } M_C = \rho V_C \tag{3.55}$$

CHAPTER 4

MONTE CARLO METHOD

4.1 Introduction

Computer simulation programs are getting more attention in calculations of statistical physics such as the study of phase transitions, and they become an important tool in learning and understanding the main principles of statistical mechanics and also thermodynamics [7], [24]–[30]. The reason why it has such an importance is because of its simplicity in the application: Not only all but the simplest models in these areas are theoretically intractable, and only approximate methods are generally able to be used. In particular, stochastic techniques called as Monte Carlo Method (MCM) simulations have also proven itself to be very powerful in its applications [31]. The MCM is simply a technique of generation and use of random numbers to solve a problem.

The MCM has long been applied as a powerful technique for performing many types of calculations which are too complicated even for a more classical approach. As the usage of powerful computers took widespread applications in the 1950s, many of theoretical investigations have been studied and practical experiences have been gained by the MCM approach. There are many fields in which MCM has been studied are as followings (see [27] and Refs. therein):

- Mathematics, in *Numerical Analysis.*
- Physics, in *Simulation of Natural Phenomena*.
- Engineering, in *Simulation of Experimental Apparatus*.
- Biology, in *Cell Simulations.*
- Statistics, in *Distribution Functions*.
- Economy, in *Modelling Stock Exchange*.

The huge and wide information about the MCM and its history can be found in internet. As a short part, we only give here that the explosive growth in the use of

Monte Carlo applications in diverse areas of physics has prompted wide investigation of new methods and of the understanding of both old and new techniques.

4.2 Determination of Pi

One of the simplest and best example for the application of the MCM is estimation of Pi or π value that is a mathematical constant related with the ratio of any circle's circumference to its diameter. If we consider a circle of radius r, then its diameter is given by 2r [30].

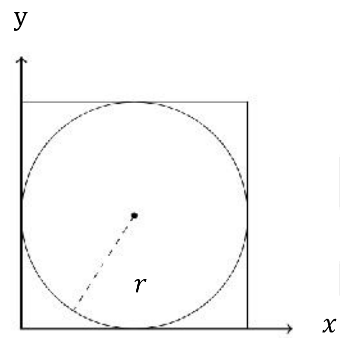


Figure 4.1 Shows the circle centered in a tight square.

Then,

$$\text{circle's circumference(C)} = 2\pi r$$

$$\text{circle's diameter(D)} = 2r$$

$$\frac{\mathrm{C}}{\mathrm{D}} = \frac{2\pi r}{2\pi r} = \pi$$

One estimate π value via using the MCM: Now let us assume a circle centered in a tight square as a shown in the Fig. 4.1. For instance, the radius of circle "*r*" gives us length side of one-quarter of square is *r* then yields the one-quarter square area is

$$A_{\boxdot} = r * r = r^2$$

where the area of circle is

$$A_{\odot} = \pi r^2$$

If we divide area of circle by r^2, we get

$$\pi = \frac{A_{\odot}}{r^2}$$

Now if we look at the circle especially on the portion S in Figure 4.2, then the area of portion S is given by

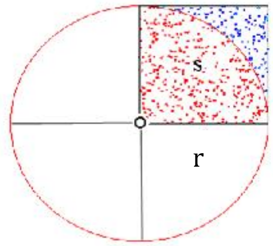


Figure 4.2 Shows the area of S within the square.

$$S = \frac{1}{4} A_{\odot}$$

Consequently

$$4S = A_{\odot}$$

That implies the area of the circle is four times to the area of the portion S. Then, substituting into to the previous equation gives us

$$\pi = \frac{4S}{r^2}$$

as shown in the Figure 4.2

$$\frac{S}{r^2} = \frac{area\ of\ {}^{1}/_{4}\ circle}{area\ of\ square} \approx \frac{n_{\odot}}{n_{total}}$$

Now we shall be using MCM to estimate ($S\ and\ r^2$) quantities: If we generate n random points in the square, we could count how many points fall inside the area of the quarter circle. The MCM program generates random points inside the square. It then controls if the point is inside the circle (it is known that it is inside the circle if $x^2 + y^2 < r^2$, where x and y are the space components of this point and r is the radius of the circle). Then the program determines how many points it's picked so far (n_{total}) and how many of them fell inside the circle ($n_{\odot}$). The basic idea of the MCM becomes clear from the dartboard method of choosing random numbers and we represent it as darts on the dartboard. We just pick out points randomly inside the square. Then one can write

$$\pi = 4\left(\frac{S}{r^2}\right) \approx 4\left(\frac{n_{\odot}}{n_{total}}\right) = 4\left(\frac{\#\ of\ hits\ within\ the\ circle}{total\ \#\ of hits\ on\ board}\right)$$

and then the value of Pi is estimated. We present our results in the following Tables 4.1 and 4.2 where "*Exp*." is Number of Experiments (iteration of the process); "*n*" is the total number of random points generated; "*T*" is total time to perform the calculation in unit of second; "Error%" is the percentage error in the process compared to the actual value of Pi, π=3.141592654..

Table 4.1 Estimation of Pi with Error % values for *Exp*. =10 and *Exp*. =100.

-	$1^{st} set\ (Exp = 10)$			$2^{nd} set\ (Exp = 100)$		
n	Pi	Error%	T(s.)	Pi	Error%	T(s.)
10	3.1999999	1.8591635788	≈ 0.	3.1720000	0.967895897	≈ 0.
10^2	3.1840000	1.3498677609	0.015	3.169600	0.8915015248	0.109
10^3	3.1184	0.7382450924	0.109	3.1501600	0.2727071060	1.029
10^4	3.14472	0.0995465279	1.014	3.1438279	0.0711532861	10.29
10^5	3.1404039	0.0378360188	9.937	3.1418955	0.0096430837	101.7
10^6	3.1412276	0.0116200166	101.4	3.1414026	0.0060470471	1060.7

Table 4.2 Estimation of Pi with Error % values for *Exp*. =200 and *Exp*. =400.

-	$3^{rd} set\ (Exp = 200)$			$4^{th} set\ (Exp = 400)$		
n	Pi	Error%	T(s.)	Pi	Error%	T(s.)
10	3.1760000	1.0952198519	0.031	3.169000	0.8724029316	0.046
10^2	3.1159999	0.8146394651	0.218	3.1603	0.5954733306	0.405
10^3	3.1366000	0.1589210995	2.059	3.143670	0.0661239899	4.087
10^4	3.1423480	0.0240434229	20.79	3.141176	0.0132624956	40.95
10^5	3.1418071	0.0068292243	200.6	3.141887	0.0093693372	428.5
10^6	3.1417108	0.0037607170	2039	3.1416173	0.0007861111	4126

Tables 4.1 and 4.2 show four sets for the calculation of Pi value and each set present six cases from 10 to 10^6 for randomly generated numbers of "*n*"; and for each set we repeat the calculation for different number of experiments for each "*n*". It can be obviously seen that the error percent in 4^{th} set is less than all of other sets. The lowest value of error percent belongs to the 4^{th} set; in contrast, the 1^{st} set where the highest value of error percent appears. For each set we repeat the same procedure for different Number of Experiments as *Exp*.=10, 100, 200 and 400. As it is seen, the percent error decreases dramatically as the *Exp*. value is increased. If one takes a look at the Tables 4.1 and 4.2 it can be seen that the time interval *T* for each "*n*" value changes gradually: In each set it is clear that the *T*-value increases by factor of

ten if "n" value is increased by power of ten. Therefore, one may here suggest to set n=10^4 for the next calculations because the error percent in the determination of Pi is quite acceptable (~0.1%) for n=10^4 and *Exp*.=10.

The first investigations in the calculation of Pi value are illustrated through the Figures 4.3 to 4.12 below where it can be observed the accuracy of outcomes increases when the number of "n" is increased for each set compared with the actual value which is equal 3.141592654. Figures 4.3 to 4.10 give us the average value of Pi with the percent error value for *Exp*.= 10, 100, 200 and 400, respectively. It is clearly seen for a constant value of "n" (say n=10^6) that the comparison between them for a good approach gives us the best value of Pi if *Exp*. is 400. However, the Figure 4.12 and 4.13 present us another information that the time required to perform such a calculation will take a great amount of time.

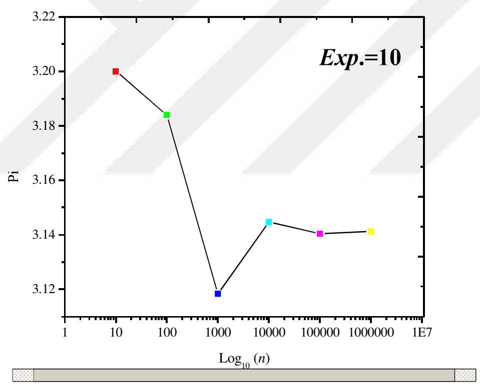


Figure 4.3 Shows the expected outcomes of Pi for *Exp*. =10.

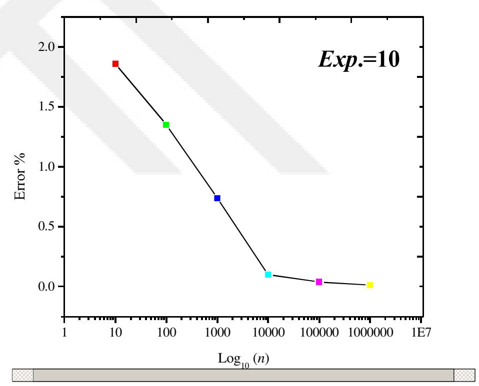


Figure 4.4 Shows the expected outcomes of Pi for *Exp*. =10.

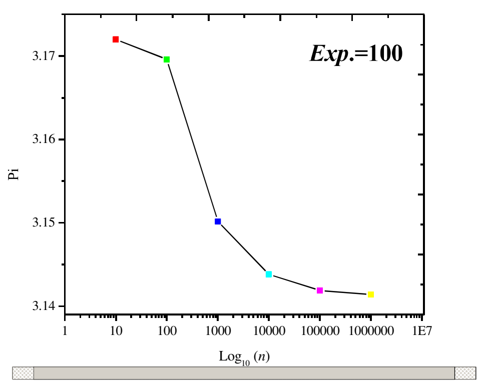


Figure 4.5 Shows the expected outcomes of Pi for *Exp*. =100.

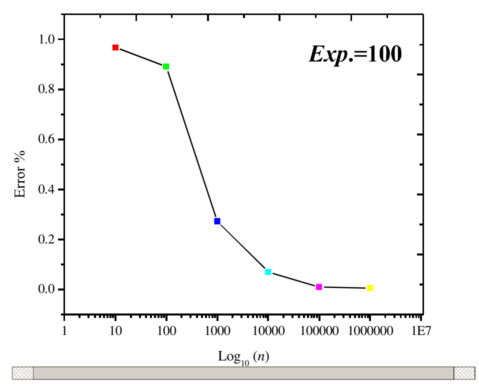
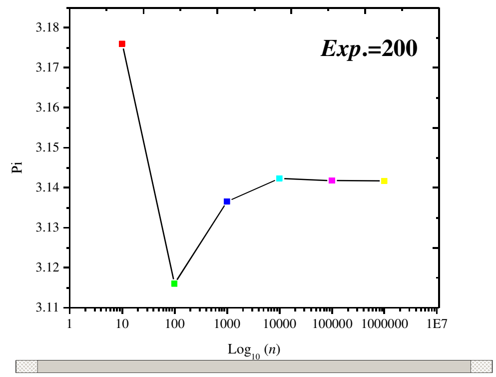


Figure 4.6 Shows the accuracy of outcomes for *Exp*. =100.



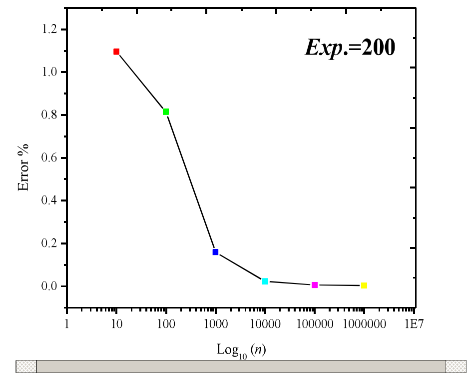
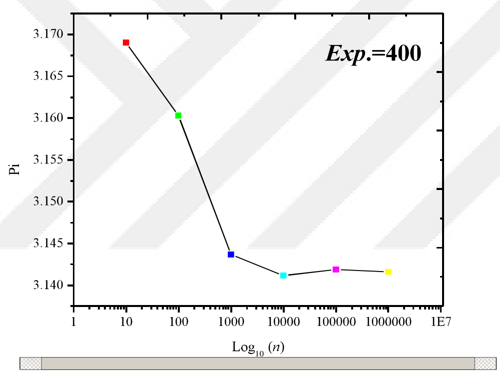


Figure 4.7 Shows the expected outcomes of Pi for *Exp*. =200.

Figure 4.8 Shows the accuracy of outcomes for *Exp*. =200.



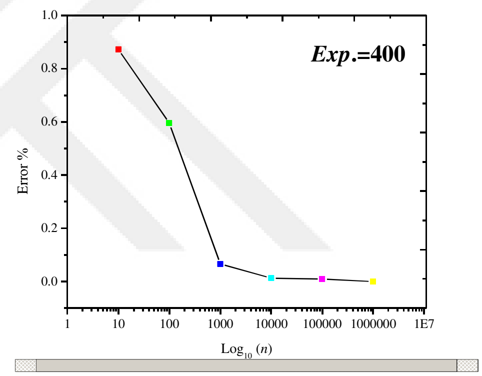
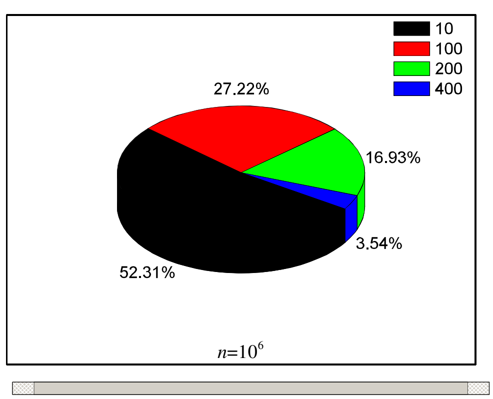


Figure 4.9 Shows the expected outcomes of Pi for *Exp*. =400.

Figure 4.10 Shows the accuracy of outcomes for *Exp*. =400



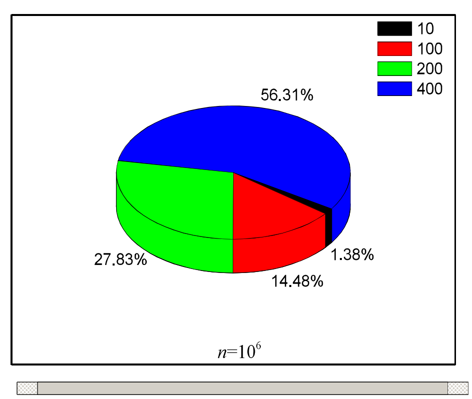


Figure 4.11 Shows the comparison of error % of Pi value for *Exp*. =10, 100, 200 and 400 (in case $n = 10^6$).

Figure 4.12 Shows the time to perform calculations for *Exp*. =10, 100, 200 and 400 (in case $n = 10^6$).

The second investigations in the calculation of Pi value are illustrated through the Figures 4.13 to 4.22 where we apply the same procedure except replace the experiment number, *Exp*., instead of number *n*.

In the following Tables 4.3 and 4.4, we repeat the running of the program but here we convert the role of the number n to experiment number, *Exp*., and the outcomes are shown.

Table 4.3 Estimation of Pi with Error % values (for *n*=10 and *n*=100).

	$1^{st} set\ (n = 10)$			$2^{nd} set\ (n = 100)$		
Exp.	Pi	Error %	*T*(s.)	Pi	Error %	*T*(s.)
10	3.08	1.9605550553	≈ 0.	3.188000	1.4771917153	0.016
10^2	3.1919999	1.6045156698	0.02	3.182800	1.3116705745	0.094
10^3	3.1471999	0.1784873797	0.11	3.1458399	0.1351972352	1
10^4	3.1442399	0.0842676534	1	3.142928	0.0425053963	10
10^5	3.1403840	0.0384726386	11	3.1412835	0.0098374813	101
10^6	3.1409436	0.0206600170	115	3.1415504	0.0013436999	1049

Table 4.4 Estimation of Pi with Error % values (for *n*=200 and *n*=400).

-	$3^{rd} set\ (n = 200)$			$4^{th} set\ (n = 400)$		
Exp.	Pi	Error%	*T*(s.)	Pi	Error%	*T*(s.)
10	3.204	1.9864875332	0.02	3.165	0.7450789771	0.05
10^2	3.1626000	0.6686846044	0.22	3.1508	0.2930789387	0.41
10^3	3.1446999	0.0989099082	2	3.1427300	0.0362028606	4
10^4	3.1432480	0.0526913127	20	3.1421650	0.0182183520	40
10^5	3.1417674	0.0055636247	208	3.1416948	0.0032514212	410
10^6	3.1415504	0.0012421582	2036	3.1416281	0.0011292492	4027

The value of the total number (n) has specified for each set and we change the value of experiments number (*Exp*.) from 10 to 10^6. It shows that there is an improvement in the value of Pi whenever the value of experiments numbers increased as shown in the 4^{th} set at $Exp. = 10^6$. Same procedures done in Tables 4.3 and 4.4 but we obtained a little bit different outcomes: The lowest value of error percent belongs to the 4^{th} set; in contrast, the 1^{st} set where the highest value of error percent appears, for each set we have repeated the process for six times to look out the effect of the experiments numbers (*Exp.*) whereas its effect can be observed when using small numbers where the error rate be is somewhat higher, to improve this issue should be using big numbers, in another hand, there are different outcomes between the $1^{st}, 2^{nd}, 3^{rd}$ and 4^{th} sets that implies there are effect for total numbers (*n*) on over the all measurements, if we take a look at the tables we can see when the total numbers (*n*) increase, the error percent will be decreasing.

We present the average approximation of Pi value in comparison with the first and second investigations as a summary for certain number of values for "*n*" and "*Exp.*" in Table 4.5.

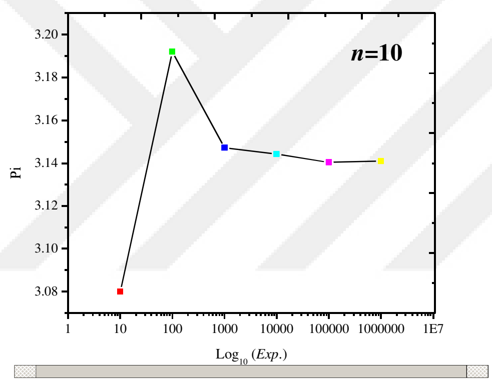


Figure 4.13 Shows the expected outcomes of Pi for *n*=10.

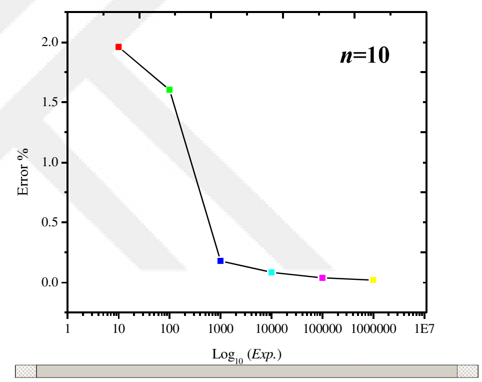


Figure 4.14 Shows the accuracy of outcomes for *n*=10.

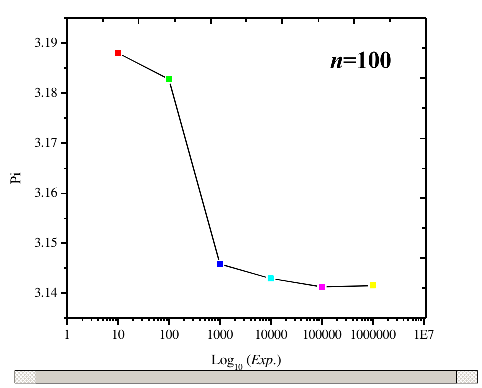


Figure 4.15 Shows the expected outcomes of Pi for *n*=100.

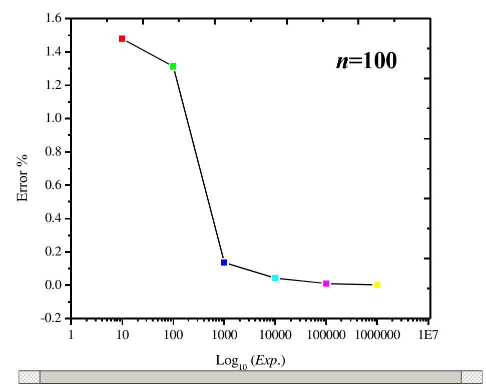


Figure 4.16 Shows the accuracy of outcomes for *n*=100.

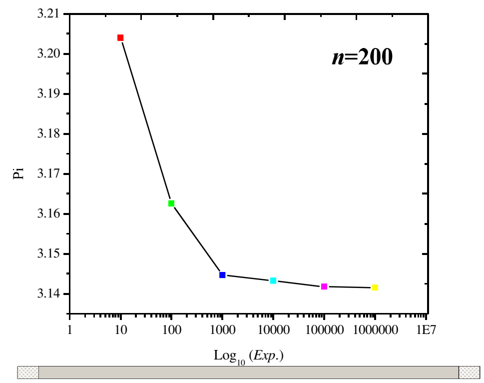


Figure 4.17 Shows the expected outcomes of Pi for n=200.

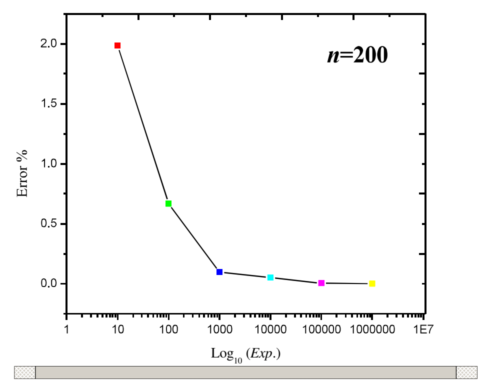


Figure 4.18 Shows the accuracy of outcomes for n=200.

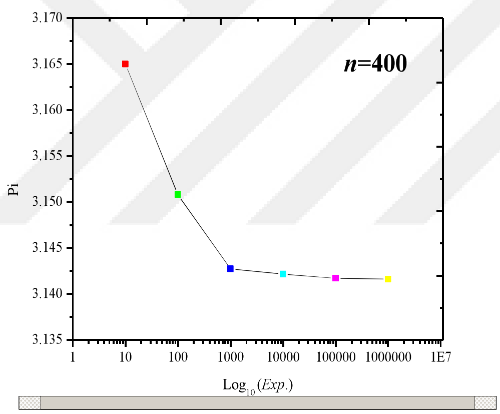


Figure 4.19 Shows the expected outcomes of Pi for n=400.

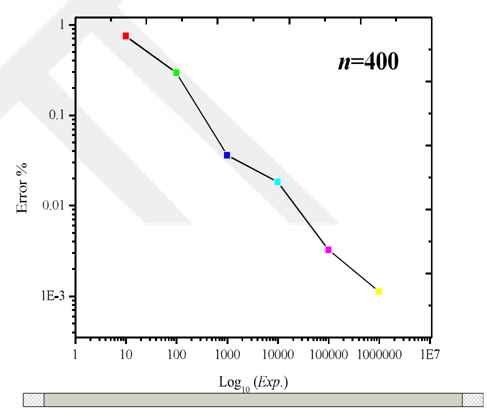
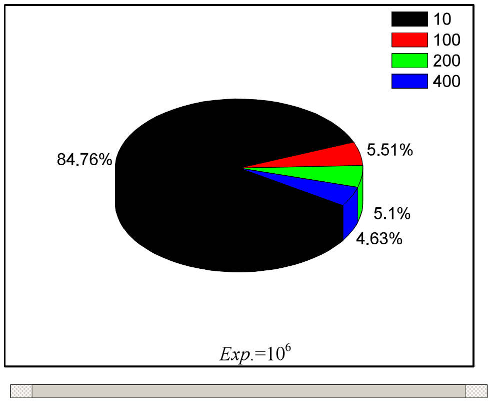


Figure 4.20 Shows the accuracy of outcomes for n=400.

The final conclusion is that it is possible to obtain a more accurate value for Pi through an increase in the experiments numbers (*Exp.*) and total numbers (n) but the difficulty is the time taken by PC to perform the calculations where it takes more time as the value of the (experiments numbers and total numbers) increases this leads us to the importance of using the PC to perform the calculations quickly and to obtain outcomes more accurate.



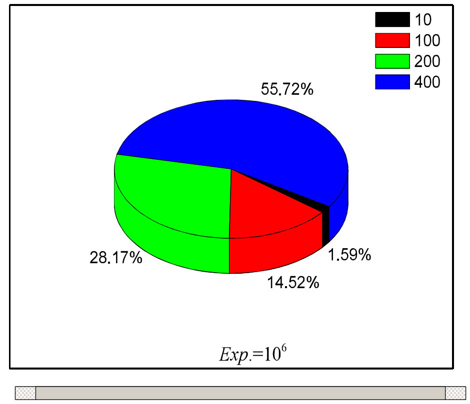


Figure 4.21 Shows the comparison of error % of Pi value for n=10, 100, 200 and 400 (in case $Exp. = 10^6$).

Figure 4.22 Shows the time to perform calculations for n=10, 100, 200 and 400 (in case $Exp. = 10^6$).

The best outcomes of Pi values is shown clearly from the Table 4.5 when the number of *Exp.* and *n* are largest among all cases and the accuracy of the outcome for Pi value is proportional to the increase in the value of *Exp.* and *n*.

Table 4.5 Comparison between the error percent of Pi value for the optimum cases.

	Exp.			*n*		
n	10^5	10^6		10^5	10^6	*Exp.*
200	0.0055636247	0.0013436999		0.0068292243	0.0037607170	200
400	0.0032514212	0.0011292492		0.0093693372	0.0007861111	400

We used a PC in this study with the following specifications:

- Windows edition: Windows 7 Ultimate.
- Processor: Intel(R) Core(TM) i5 CPU M520 @ 2.40GHz.
- Installed memory (RAM): 4.00 GB (3.80 GB usable).
- System type: 64-bit Operation System.
- Hard disk size: 500 GB.
- Adapter type: Intel(R) HD graphics.
- Total available graphics memory: 1696 MB.
- Dedicated video memory: 64 MB.
- System video memory: 0 MB.
- Shared system memory: 1632 MB.

CHAPTER 5

CALCULATION OF CRITICAL MASS

5.1 Introduction

In a chain reaction, neutrons which are emitted in a fission reaction collide with other U-235 nuclei. If these nuclei absorb neutrons, then they become highly unstable and then may rapidly undergo another fission reaction emitting more neutrons which are as trigger for more fission reactions, and so on. Each phase of this kind of a process is called as "generation". If one assumes that there are two neutrons in average emitted in fission, and if each emitted neutron may induce another fission reaction, then one start to count N spontaneous fissions resulting in 2N induced fissions after one generation; $4N$ after two generations; and so on, and finally $2^{\mathrm{n}}N$ after n generations. Therefore, the number of induced fissions will dramatically grow in exponent and it will reach finally $2^{30} \approx$ one billion times the initial number of spontaneous fissions only after 30 generations [32]. In the view previous discussion, one possibly asks why a chain reaction does not always result from spontaneous fissions. It is obviously related with the notion of critical mass [33] that is the possible smallest mass of fissile element, such as uranium or another fissionable material in which a self-sustaining chain reaction may take place. Because of small size of uranium nuclei, a neutron emitted in a nuclear fission reaction has to move, on the average, certain distances such as the order of some centimeters just before interacting with other fissile nuclei in medium and then inducing them to make fission. Thus, for a small piece of fuel element even if two neutrons are possibly emitted during the spontaneous fission, one of them or possibly both of them may leave the piece before reacting with another fissile nucleus. In such a case, the average number of induced fissions by spontaneous fissions would possibly be number less than two. If we define the quantity:

$$f_s(\mathrm{k}) = N_{in}/\, N$$

where N_{in} is the number of fissions induced by neutrons emitted in N fissions during the preceding generation then one shall refer to f_s as the *multiplication* *factor* "k" or "*survival fraction* "f_s". As mentioned before, if it starts with N fissions in the first generation, there will be $(f_s N)$ fissions in the next generation; and then, one gets $(f_s{}^2 N)$ fissions in the one after that; and finally one has $f_s{}^n N$ fissions at the end of n^{th} generation. If and only if $f_s \geq 1$, there will exponentially be growth in the released energy resulting from generation to generation. The value of f_s for a particular piece of fuel is determined by its mass, shape, and also its purity. If a piece of uranium for which $f_s = 1.0$, then it is said to have a critical mass of fissile material. If a piece of uranium has a mass greater than M_C, it may then spontaneously undergo a chain reaction and possibly may cause a nuclear explosion [34]. To create such an explosion, one just need to bring two pieces of uranium together whose combined mass then will exceed M_C. Determining the value of the critical mass theoretically is extremely important since the experimental determination has a bit of risk. At the beginning of the nuclear age, there were many scientists who actually attempted such experimental processes which were called "tickling the dragon's tail." [35]

The starting point of the program is firstly to define the physical system of interest, its variables, parameters of the material, and the values of physical quantities, such as shape [36]. We also define the parameters that control our simulation such as the number of neutrons per fission, the number of experiments, and the desired precision of the results if possible.

The next step in the program is a preliminary calculation of each case to provide enough information about the system in problem which will be useful for us to optimize the efficiency of the simulation.

5.2 Calculation of the Critical Mass for a Bare Rectangular Reactor

As a first application we use the MCM code for a hypothetical rectangular block of fissile element to find the survival fraction for a range of masses and shapes (recall that a block has the critical mass provided the survival fraction has the value $f_s = 1.0$). The procedure we shall use to find the value of f_s for a block of specified size and shape involves generating a large number (N) of simulated random fissions, and keeping a count of the number (N_{in}) of induced fissions which are caused by the emitted neutrons. The first step in generating a random fission is to choose the location of the nucleus undergoing fission to be a random point (x_0, y_0, z_0), lying within the boundaries of the piece of uranium (see Fig. 5.1). If we assume that the

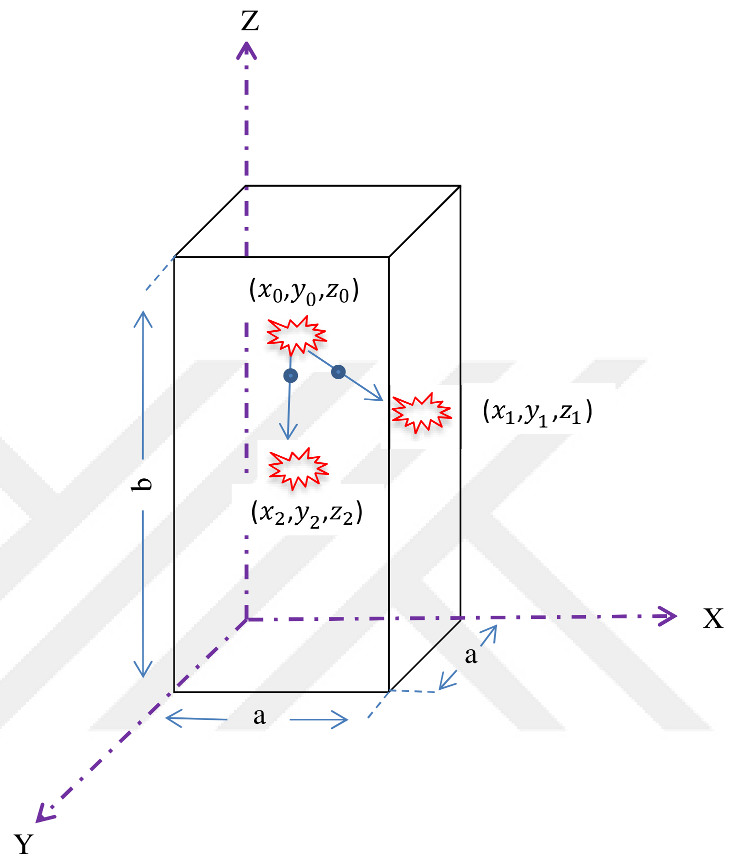


Figure 5.1 A fission is assumed to occur at a randomly located point giving rise to two neutrons travelling along random directions indicated by the dotted lines.

piece of uranium is a rectangular block of dimensions $a \ x \ a \ x \ b$ then we must choose random values for the coordinates $x_0, y_0 \ and \ z_0$, subject to the conditions:

$$\begin{aligned} \left(-\frac{a}{2}\right) &\leq x_0 \leq \left(+\frac{a}{2}\right) \\ \left(-\frac{a}{2}\right) &\leq y_0 \leq \left(+\frac{a}{2}\right) \\ \left(-\frac{b}{2}\right) &\leq z_0 \leq \left(+\frac{b}{2}\right) \end{aligned} \tag{5.1}$$

The only fission fragments we concerned are the neutrons, since the heavy nuclear fragments play no part in the chain reaction mechanism. The two neutrons emitted during the fission process may travel in many directions. A direction in three dimensions can be specified by two angles: θ the polar angle, and ϕ , the azimuth. If the emitted neutrons have an “isotropic" distribution, i.e., all directions are equally likely, then the probability of a neutron emitted from the point (x_0, y_0, z_0) hitting any area on a surrounding unit sphere depends only on the size of the area. This implies that the azimuth ϕ is uniformly distributed between 0 and 2π, that $\cos\theta$ is uniformly distributed between -1 and 1. Note that it is $\cos\theta$ not θ itself, which is uniformly distributed due to the fact that equal intervals in $\cos\theta$ contain the same surface area on a sphere of unit radius. Whether an emitted neutron hits another nucleus before leaving the block depends only on the distance along its line of flight to the boundary of the block. We shall assume (unrealistically) that a neutron emitted during fission can hit another nucleus after it travels any distance between 0 and 1 centimeter, with equal probability. For example, if a neutron travels along a direction such that it would leave the block after traveling only 0.3 cm, then there is a 30% chance of it hitting a nucleus in the block. Our procedure, therefore, is to choose a random number between 0 and 1 for d, the distance traveled by each neutron. Since the neutron starts at the point (x_0, y_0, z_0) and travels along a direction (θ, ϕ), we can find the coordinates of the point (x_1, y_1, z_1) where the neutron would hit another nucleus using the geometrical relations.

$$
\begin{aligned}
x_1 &= x_0 + d\ \sin\theta\ \cos\phi \\
y_1 &= y_0 + d\ \sin\theta\ \sin\phi \\
z_1 &= z_0 + d\ \cos\theta
\end{aligned}
\tag{5.2}
$$

whether the neutron actually hits a nucleus at the point (x_1, y_1, z_1) and causes it to fission depends on whether the point lies within the block.

To calculate the survival fraction, we need only generate a large number of random fissions (*N*) and keep a count of the number of neutron endpoints (N_{in}) which lie inside the block. To generate each random fission, we need nine random numbers $r_1, r_2, \ldots, r_9$, which lie between 0 and 1. The nine quantities needed for each random fission are obtained from the random numbers $r_1, r_2, \ldots, r_9$, according to the following equations:

$$
\left.\begin{array}{l}
x_0 = a\left(r_1 - \frac{1}{2}\right) \\
y_0 = a\left(r_2 - \frac{1}{2}\right) \\
z_0 = b\left(r_3 - \frac{1}{2}\right)
\end{array}\right\} \left[\begin{array}{c} coordinates\ of\ nucleus \\ fission \end{array}\right]
$$

$$
\left.\begin{array}{l}
\phi = 2\pi r_4 \\
\cos\theta = 2\left(r_5 - \frac{1}{2}\right)
\end{array}\right\} \left[\begin{array}{c} two\ angles\ for\ one \\ emitted\ neutron \end{array}\right] \quad (5.3)
$$

$$
\left.\begin{array}{l}
\phi' = 2\pi r_6 \\
\cos\theta' = 2\left(r_7 - \frac{1}{2}\right)
\end{array}\right\} \left[\begin{array}{c} two\ angles\ for\ other \\ emitted\ neutron \end{array}\right]
$$

$$
\left.\begin{array}{l}
d = r_8 \\
d' = r_9
\end{array}\right\} \left[\begin{array}{c} distance\ traveled\ by \\ each\ neutron \end{array}\right]
$$

These formulas insure that each of the nine parameters will lie within the proper range. For each neutron from a random fission we need to calculate the neutron endpoint from Eq. (5.1), and then test whether the point is inside or outside the block. The survival fraction f_s is then given by $f_s = N_{in}/N$. In using the Monte Carlo method to find the *survival fraction* f, we are actually integrating a function F of nine variables:

$$F = F(x_0, y_0, z_0, \phi, \theta, d, \phi', \theta', d')$$

which represents the number of fissions induced by two emitted neutrons for particular values of the variables $x_0, y_0, \ldots, d'$. The value of F is zero, one, or two, depending on these variables. In order to obtain the survival fraction f_s, we, must integrate the function F over all nine variables. The advantages of the Monte Carlo technique over conventional integration techniques are quite apparent in a case such as this. In order to evaluate a nine-dimensional integral using a finite sum, each of the nine variables must be allowed to take on some number of values. If only two values are used for each variable, it becomes necessary to evaluate the function at $2^9 = 512$ points.

For simplicity we calculate the critical mass of rectangular blocks of dimension $a\ x\ a\ x\ b$. To calculate the critical mass for a given shape we want to keep the ratio $(S = a/b)$ fixed and vary the mass of the block, M, until the survival fraction f_s has the value 1.0. We can then vary the ratio $S = a/b$, to find the critical mass for each shape. It is assumed that the block has unit density (g/cm^3) so that its dimensions a and b (cm) can easily be found in terms of S and M (even for hypothetical shape).

$$a = (\mathrm{M} * S)^{1/3}$$
$$b = \left(\frac{\mathrm{M}}{S^2}\right)^{1/3} \tag{5.4}$$

The inputs in our program are:

N = number of randomly generated neutrons.

M = mass of the rectangular block.

S = ratio of length to thickness (shape of block).

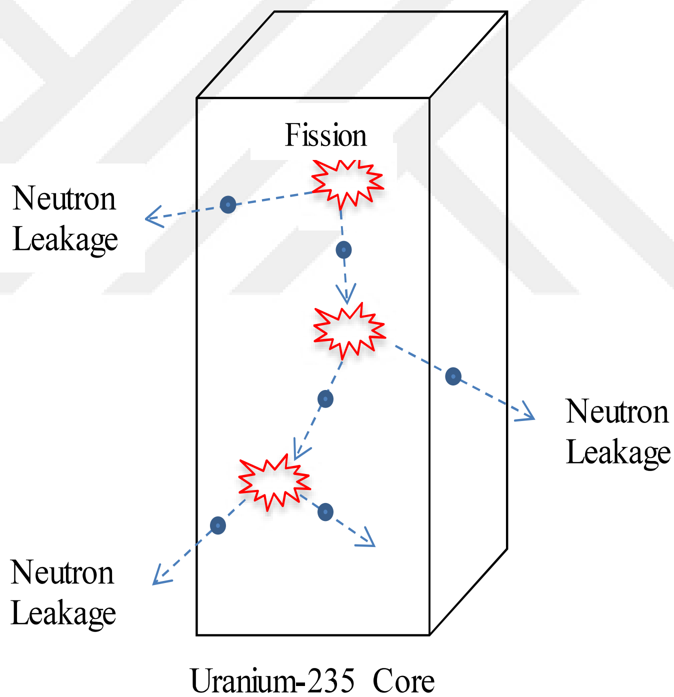


Figure 5.2 Shows the virtual fission processes inside the Cartesians coordinate system.

Running the program by using a range of values for the number of randomly generated neutrons one can calculate the minimum critical mass/size in any geometry. Because the accuracy of the calculation can be increased by using a higher value of N, we first investigate a relation, if exists, among parameters M, S, and N used as indicative factors of the statistical fluctuations presented in our Monte Carlo calculation, as shown in Table 5.1.

Table 5.1 Shows the relation between the number of initial neutrons *N* and the survival fraction for the rectangular blocks.

1^{st} set ($S = 1$ and $\mathrm{M} = 1$ are constants)						
N	10^2	10^3	10^4	10^5	10^6	10^7
f_s	0.98	0.876	0.8887	0.89652	0.895712	0.895665
	0.80	0.867	0.8835	0.89657	0.895789	0.895789
	1.02	0.899	0.8933	0.89416	0.895131	0.895478
	0.95	0.916	0.8894	0.89689	0.897115	0.895496
	0.92	0.915	0.8941	0.89231	0.895246	0.895299
	0.78	0.907	0.9030	0.89351	0.896667	0.895235
	0.93	0.897	0.8888	0.89557	0.894426	0.895358
	0.75	0.880	0.8887	0.89472	0.895771	0.895251
	0.98	0.921	0.8837	0.89323	0.896237	0.895426
	0.86	0.929	0.9025	0.89337	0.894728	0.895507
$\bar{f_s}$	0.897	0.9007	0.89157	0.894685	0.895682	0.89545
$T(S.)$	0.156	1.10760	10.9824	111.9463	1077.545	10900.757

Table 5. 2 Shows the relation between the mass M and the survival fraction for the rectangular blocks.

	2^{nd} set ($N = 10^6$ and $\mathrm{S} = 1$ are constants)						
M	0.1	0.5	1.0	1.5	2	8	16
f_s	0.417120	0.708260	0.895712	0.98202	1.05220	1.34947	1.46378
	0.414960	0.708160	0.895789	0.98380	1.05554	1.34802	1.47017
	0.414990	0.712010	0.895131	0.98618	1.05647	1.34572	1.46916
	0.415320	0.712820	0.897115	0.98274	1.05786	1.34940	1.46560
	0.413290	0.706270	0.895246	0.98403	1.05748	1.34998	1.46658
	0.412680	0.709150	0.896667	0.98401	1.05866	1.34868	1.46628
	0.415590	0.708110	0.894426	0.98344	1.06063	1.35077	1.46519
	0.413930	0.708840	0.895771	0.98472	1.04900	1.34813	1.46278
	0.415960	0.707620	0.896237	0.98418	1.05645	1.34764	1.46507
	0.415590	0.709220	0.894728	0.98679	1.05656	1.34851	1.47142
$\bar{f_s}$	0.414943	0.709046	0.895682	0.98419	1.05608	1.34863	1.46660
$T(s.)$	1077.53	1160.039	1077.545	1108.7	1116.98	1122.92	1122.77

In another case, we can search for the relation among the parameters M, S and *N* as following: One can set $N = 10^6$ and $\mathrm{S} = 1$ for all runs, and then search for the critical mass value for which the survival fractions becomes/reaches "1.0". The results are given in Table 5.2. Since the certain amount of fissile material is needed to reach criticality, a condition where the number of neutrons generated through fission balances out the number of neutrons lost through leakage. While the minimum mass required reach at criticality condition is a function of the geometry, the optimal shape to obtain the minimum amount of fissile material to make the reactor critically is to be determined. From Table 5.2, one can conclude that the minimum critical mass in this geometry is between M=1.5 and M=2.0 because the value of survival fraction is about "1.0" there. Therefore, we need to search for the minimum mass depending on the shape parameter at which f_s=1.

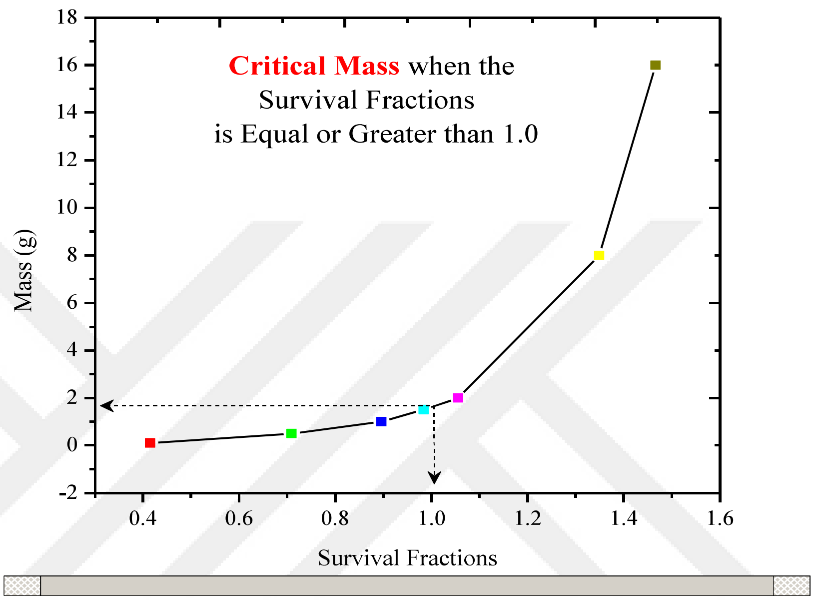


Figure 5.3 Shows the effect of mass M of the block on the survival fraction for the rectangular blocks.

It can be understood how the mass effect on the survival fraction f_s for the certain values of mass (M=0.1, 0.5, 1, 1.5, 2, 8 and 16) where it shows that one could not obtain case critically for the (M=0.1, 1 and 1.5) as a consequence, lead to increase the value of the mass (M=2, 8 and 16) from which obtains the survival fractions are greater than one, so an amount of fissile material is needed to reach criticality. In short, the critical mass when survival fraction is equal or greater than one, one need to calculate the critical mass for non-cubic rectangular blocks and need to repeat the procedure via using certain values of S. We used S=0.1, 0.5, 1.0, 1.5, 2.0., 8.0 and 16. We have found the mass corresponding to each of these shapes as shown in the Table 5.3.

Table 5.3 Shows the relation between the ratios of the dimension S and the survival fraction for the rectangular blocks.

	3[rd] set ($N = 10^6$ and M = 1 are constants)						
S	0.1	0.5	1.0	1.5	2	8	16
f_s	0.59333	0.83839	0.895712	0.86717	0.84029	0.59258	0.45720
	0.60203	0.83717	0.895789	0.86393	0.83499	0.59015	0.45949
	0.59678	0.83897	0.895131	0.86696	0.83323	0.59511	0.45592
	0.59575	0.83666	0.897115	0.86606	0.83097	0.59166	0.45710
	0.59409	0.83948	0.895246	0.86712	0.83959	0.5924	0.45666
	0.59892	0.83483	0.896667	0.86542	0.83666	0.59062	0.45738
	0.59544	0.83753	0.894426	0.86762	0.83707	0.58934	0.45629
	0.59372	0.83747	0.895771	0.86465	0.83567	0.59073	0.45842
	0.59349	0.84017	0.896237	0.86315	0.83951	0.58791	0.45771
	0.59588	0.84036	0.894728	0.86577	0.83795	0.59320	0.45602
$\bar{f_s}$	0.595943	0.83810	0.895682	0.86578	0.83659	0.59137	0.45721
$T(s.)$	1048.248	1103.72	1077.545	1099.85	1108.62	1124.82	1130.92

The effect of changing the shape clearly seen in Figure 5.4.

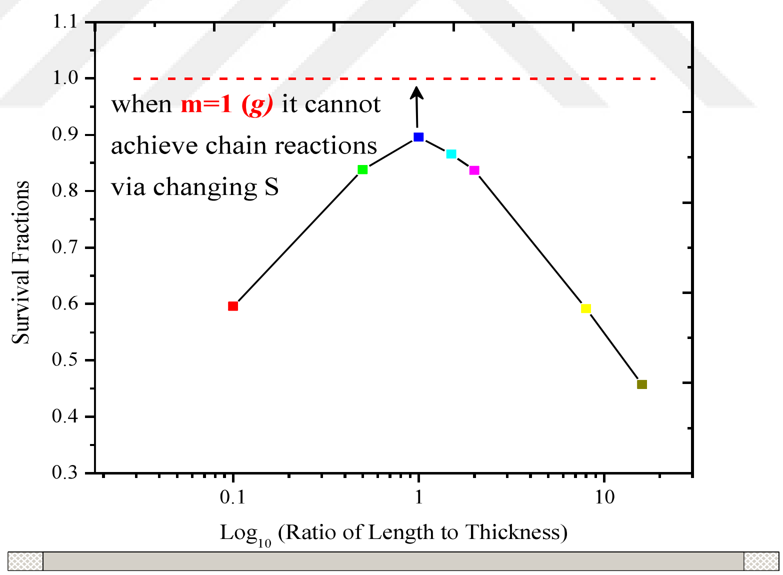


Figure 5.4 Shows the effect of dimensions of the block S on the survival fraction for the rectangular blocks.

In Table 5.3 it is clearly seen that the highest point of the survival fraction for the given geometry is about S=1 and it implies that one cannot reach to the critical case via changing the shape of block S, so the mass must be increased to make the survival fractions f_s is equal or greater than one. To know what the critical mass is for each case, the ratio of length to thickness is required to be critically through the survival fractions be equal or greater than one. Therefore, we present the minimum critical mass for each shape, S=0.1, 0.2, 0.3…. etc., for N=10^4 random points generated in total as shown in the Table 5.4.

Table 5.4 The relation among the shape S, the Mass M and the survival fraction for the rectangular blocks.

$N = 10^4$						
S	M	f_s		S	M	f_s
0.1	6.28	1.00253		2.6	2.38	1.00144
0.2	3.46	1.00211		2.7	2.47	1.00286
0.3	2.55	1.00147		2.8	2.52	1.00146
0.4	2.18	1.00600		2.9	2.6	1.00211
0.5	1.93	1.00301		3.0	2.70	1.00069
0.6	1.75	1.00137		3.1	2.73	1.00000
0.7	1.69	1.00300		3.2	2.84	1.00255
0.8	1.62	1.00026		3.3	2.95	1.00086
0.9	1.62	1.00055		3.4	3.07	1.00299
1.0	**1.61**	**1.00069**		3.5	3.13	1.00003
1.1	1.62	1.00338		3.6	3.23	1.00103
1.2	1.63	1.00058		3.7	3.28	1.00043
1.3	1.66	1.00605		3.8	3.39	1.00251
1.4	1.68	1.00099		3.9	3.48	1.00123
1.5	1.70	1.00083		4.0	3.58	1.00022
1.6	1.79	1.00601		4.1	3.66	1.00239
1.7	1.81	1.00049		4.2	3.77	1.00136
1.8	1.86	1.00177		4.3	3.90	1.00181
1.9	1.95	1.00404		4.4	4.02	1.00151
2.0	1.98	1.00075		4.5	4.08	1.00053
2.1	2.05	1.00067		4.6	4.22	1.00307
2.2	2.12	1.00125		4.7	4.31	1.00316
2.3	2.16	1.00163		4.8	4.43	1.00251
2.4	2.25	1.00332		4.9	4.56	1.00207
2.5	2.32	1.00144		5.0	4.61	1.0027

In order to calculate the minimum critical mass, we write a code to give us the minimum mass value for each S through the calculation of the survival fraction if it is equal or greater than 1. In Table 5.4 we give our results for the minimum mass corresponding to each shape from S=0.1 to 5.0. When S=1, we get the smallest critical mass and it is seen there is a clear effect of the shape of rectangular blocks to make the reactor critical. As shown in Table 5.4, the mass value changes from higher to lower for S=0.1 to S=1.0 and then it increases gradually. For a three specific cases for S value (a $< b, a = b$ and $a > b$), one can show this relation in the following Figure 5.5.

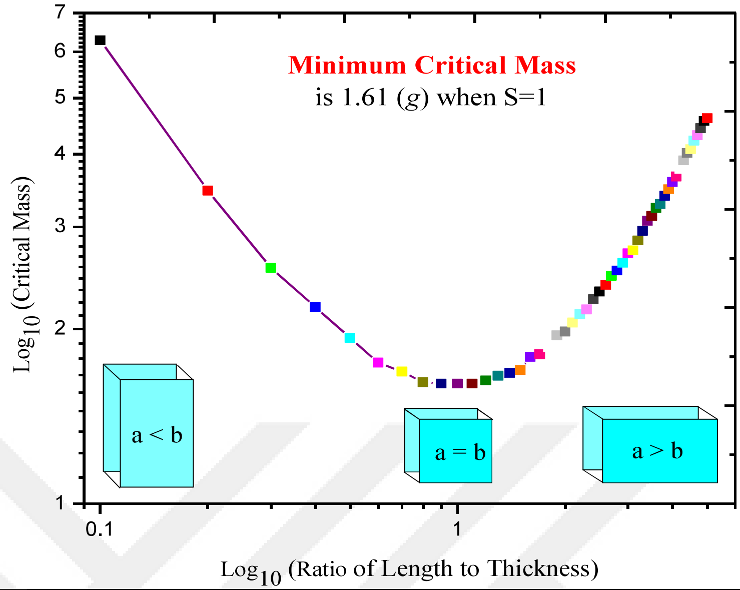


Figure 5.5 Shows the critical mass for each shape of rectangular block including a cubic block when $S = a/b = 1$ (It should be noted that f_s is greater than 1).

The rectangular parallelepiped with least volume is cube as it might be expected. It is noted that we found $S = 1$ as shown in Fig. 5.5 that yields the smallest critical mass. To calculate the minimum ratio of the length to the thickness, we can consider $a = c \neq b$, so it can be assumed that the rectangular of length "a" and thickness "b".

Since the volume V of the rectangular is

$$V = a^2\, b$$

and the length to thickness ratio (a/b) is assumed to be

$$S = \frac{a}{b} \quad \Longrightarrow \quad a = S\, b$$

Hence we may write

$$V = (S\, b)^2\, b \quad \Longrightarrow \quad b = \left(\frac{V}{S^2}\right)^{1/3}$$

The buckling of critical reactor for a rectangular is given by

$$B^2 = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2$$

If we consider $c = a \neq b$

$$B^2 = \left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{a}\right)^2$$

Substituting $a = S\, b$ in the last equation we get

$$B^2 = \left(\frac{\pi}{S\,b}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{S\,b}\right)^2$$

$$B^2 = \left[\left(\frac{\pi}{S}\right)^2 + \left(\frac{\pi}{1}\right)^2 + \left(\frac{\pi}{S}\right)^2\right] * \frac{1}{b^2}$$

Then one writes

$$B^2 = \left[\left(\frac{\pi}{S}\right)^2 + \left(\frac{\pi}{S}\right)^2 + (\pi\,)^2\right] * \frac{1}{\left(\frac{V}{S^2}\right)^{2/3}}$$

$$B^2 = \left[\,2 * (\pi)^2 * S^{-2} + (\pi\,)^2\right] * \frac{S^{4/3}}{(\,V\,)^{2/3}}$$

For the minimum buckling with constant *V*, we have to derivative with respect to S

$$\frac{d}{dS}B^2 = \left\{\frac{1}{(\,V\,)^{2/3}} * \left[\,2 * (\pi)^2 * S^{-2} * S^{4/3} + (\pi\,)^2 * S^{4/3}\right]\right\}$$

$$\frac{d}{dS}B^2 = \left\{\frac{1}{(\,V\,)^{2/3}} * \left[-\frac{4}{3} * (\pi)^2 * S^{-5/3} + \frac{4}{3}(\pi\,)^2 * S^{1/3}\right]\right\} = 0$$

$$-S^{-5/3} + S^{1/3} = \frac{-1 + S^2}{S^{5/3}} = 0$$

The result is found to be

$$S = 1$$

The final equation implies a=b=c, so the minimum critical volume gives us a cubic shape. The geometry of the reactor is specified, the buckling can then be determined from the appropriate formula for B^2. Thus, for a cubic reactor we have the condition:

$$B = \pi\sqrt{3}/a$$

5.3 Calculation of the Critical Mass for a Bare Cylindrical Reactor

Cylindrical coordinates are results of generalization of polar coordinates in two dimensions to three dimensions by defining a height (z) axis. In the literature, there are different notations used for two coordinates; r and θ. Both symbols, r and ρ, are used to show the radial coordinate and either θ or ϕ to the azimuthal coordinates. $Arfken$ (1985) uses (ρ, ϕ, z) while $Beyer$ (1987) uses (r, θ, z). In this work, the notation (r, θ, z) is used [37].

We shall determine the critical mass of cylindrical block with its dimensions $(r * h)$. To find the critical mass of a given shape it is to keep the ratio $(S = h/r)$ fixed and then change the mass of the block, M, until the survival fraction f_s has the value 1.0. One can then vary the ratio $(S = h/r)$, to calculate the critical mass for each shape. The dimensions h and r can then be easily determined in terms of S and M.

$$r = \left(\frac{\mathrm{M}}{\pi * \mathrm{S}}\right)^{1/3}$$
$$h = \left(\frac{\mathrm{M} * \mathrm{S}^2}{\pi}\right)^{1/3} \quad (5.5)$$

The cylindrical coordinates are (r, θ, z) considering $z = h$, whereas in terms of the Cartesian coordinates (x_0, y_0, z_0) are

$$x_0 = r \cos\theta$$
$$y_0 = r \sin\theta \quad (5.6)$$
$$z_0 = h$$

where $x_0, y_0,$ and z_0 are initial coordinates of the fission which emitting a neutron inside the boundaries of the blocks shown in Figure 5.6.

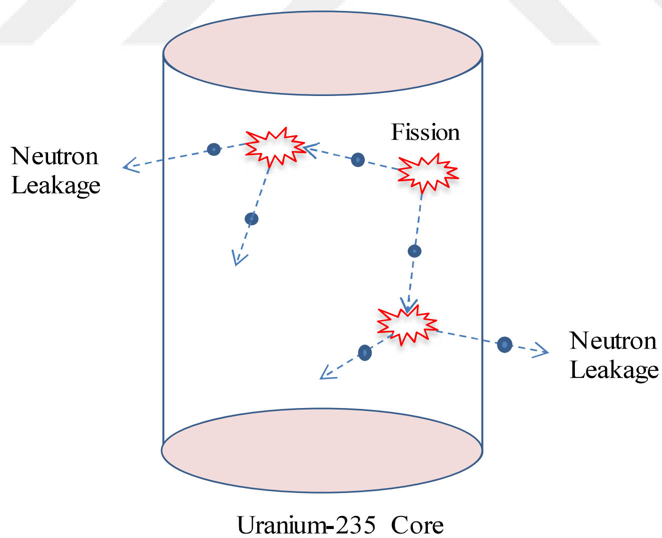


Figure 5.6 Shows the virtual fission processes inside the cylindrical coordinates systems.

By running our program for $\mathrm{S} = h/r$ using a range of values for the number of randomly generated neutrons of N, we present our results from Table 5.5 to Table 5.8. In Table 5.5 we present the effect of "N" for constant values of S and M. If M and S are kept constant, the effect of N is not obvious in the calculation of "f_s" parameter.

Table 5.5 Shows the relation between the number of initial neutrons *N* and the survival fraction for the cylindrical.

1st set (S=1 and M=1 are constants)						
N	10^2	10^3	10^4	10^5	10^6	10^7
f_s	1.	0.926	0.9533	0.94424	0.945162	0.945761
	1.01	0.895	0.9335	0.94829	0.944673	0.945918
	0.99	0.969	0.9398	0.95008	0.94639	0.945648
	0.82	0.968	0.9378	0.94717	0.945653	0.945252
	0.95	0.953	0.9545	0.94569	0.945749	0.945371
	0.97	0.952	0.9384	0.94269	0.945933	0.945952
	1.03	0.951	0.944	0.94507	0.945596	0.945776
	0.83	0.919	0.9564	0.94571	0.946023	0.945521
	0.95	0.924	0.9404	0.94889	0.94638	0.945372
	0.89	0.935	0.9437	0.94774	0.947706	0.945649
$\bar{f_s}$	0.944	0.9392	0.94418	0.946557	0.9459265	0.945622
$T(s.)$	0.145	1.0764	10.327	105.425	968.0954	10094.32

We set S=1 and N=10^6 to see the effect of M in the calculation. In Table 5.6 it is clear that the survival fraction increases as M increases. It is an expected result because all neutrons in higher mass are absorbed. Outcomes are given in Table 5.6.

Table 5.6 Shows the relation between the mass M and the survival fraction for the cylindrical blocks.

	2nd set ($N = 10^6$ and S = 1 are constants)						
M	0.1	0.5	1.0	1.5	2	8	16
f_s	0.444541	0.760047	0.945162	1.06297	1.14433	1.47582	1.59049
	0.443024	0.759841	0.944673	1.06186	1.14513	1.47445	1.59219
	0.444184	0.759395	0.94639	1.06259	1.14441	1.47454	1.5921
	0.443794	0.759514	0.945653	1.06253	1.14512	1.47428	1.59215
	0.4434	0.758613	0.945749	1.0623	1.14577	1.47464	1.59171
	0.443961	0.758812	0.945933	1.0616	1.1436	1.47465	1.59233
	0.443843	0.759542	0.945596	1.06142	1.14482	1.47513	1.59187
	0.444416	0.76083	0.946023	1.06188	1.1433	1.47452	1.59185
	0.444247	0.759885	0.94638	1.06191	1.14538	1.47395	1.59272
	0.445321	0.758622	0.947706	1.0613	1.14409	1.475689	1.59201
$\bar{f_s}$	0.444073	0.75951	0.945926	1.06204	1.14459	1.474766	1.59194
$T(s.)$	1036.51	1029.87	968.0954	1075.95	1071.27	1084.28	1087.45

The effect of the increased mass is clearly seen by f_s value increased notably. Since the number of target nuclei increases by M, then the number of neutrons striking and fissioning the target also increase. Figure 5.7 shows us a clear picture of the situation.

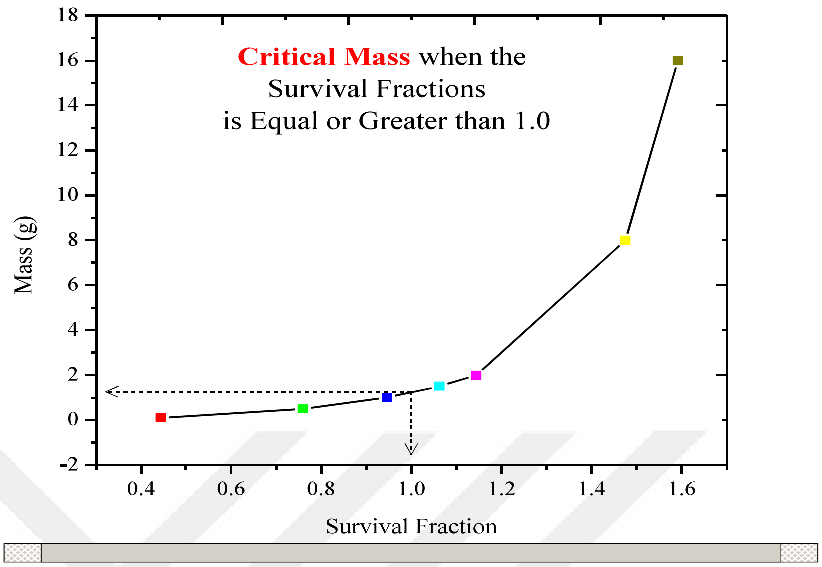


Figure 5.7 Shows the effect of mass M of the block on the survival fraction for the cylindrical blocks.

The effect of S in the determination of M is shown in Table 5.7. It is obvious that the survival fraction value increases for range of S=0.1 to S=1.5, and then it decreases for S=2 to S=16. So, there must be a value for S between 1.5 and 2.0 to approach the critically condition for M=1.

Table 5.7 Shows the relation between the ratios of the dimension S and the survival fraction for the cylindrical blocks.

	3rd set ($N = 10^6$ and M $= 1$ are constants)						
S	0.1	0.5	1.0	1.5	2	8	16
f_s	0.473204	0.83302	0.945162	0.974038	0.973057	0.78968	0.66723
	0.473037	0.83327	0.944673	0.973834	0.972689	0.79131	0.66646
	0.473429	0.83118	0.94639	0.975304	0.972443	0.78984	0.66652
	0.474	0.83428	0.945653	0.974584	0.971732	0.79022	0.66744
	0.474007	0.83389	0.945749	0.974453	0.971965	0.79085	0.66776
	0.471869	0.83301	0.945933	0.974003	0.973622	0.78974	0.66801
	0.472911	0.83306	0.945596	0.973749	0.972911	0.79062	0.66661
	0.473482	0.83297	0.946023	0.974984	0.972269	0.78908	0.66716
	0.473736	0.83359	0.94638	0.973228	0.972172	0.79121	0.66655
	0.473801	0.83354	0.947706	0.974169	0.970597	0.79045	0.66748
$\bar{f_s}$	0.473347	0.83318	0.945926	0.974234	0.972345	0.79030	0.66712
$T(s.)$	1051.29	1074.51	968.0954	1060.76	1061.789	1007.06	1041.11

The effect of the increase in the ratio of height to the radius is shown clearly by increasing its value, notably under the fixed condition for the Mass (M) and the number of randomly generated neutrons (*N*) in Table 5.7. Additionally, Figure 5.8 gives us a clear idea for the condition. There is critic value of *S* between 1.5 and 2.0.

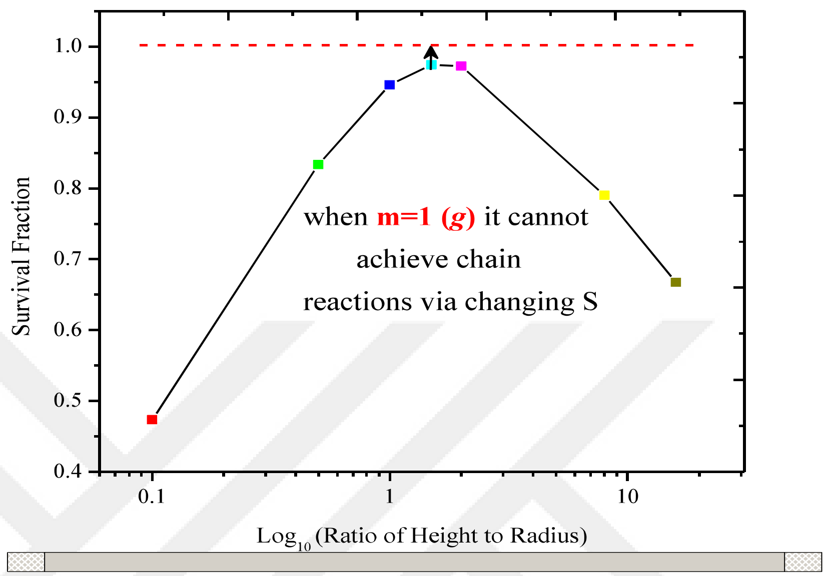


Figure 5.8 Shows the effect of dimensions of the block S on the survival fraction for the cylindrical blocks.

It is clear that the highest value of the survival fraction approaching "1" is for the condition of S between S=1.5 and S=2. That implies we cannot reach to the critical case via changing the shape of block S anymore. As shown in top of the Table 5.7 the mass equal to one for all outcomes so that the mass must be increased to make the survival fractions f_s is equal or greater than one for constant value of S.

In the case of the cylindrical block, we have three parameters (number of randomly generated neutrons "*N*", the mass of the cylindrical block "M" and the ratio of length to the thickness "S") as in the case of the rectangular parallelepiped and spherical. For each, case we keep two parameters and let the other to see the effect for each one on the survival fraction f_s, in order to determine what the critical mass is for each case of the S to the radius and to know where the exact critical dimensions is existing it is required to run the code for the critically condition through the survival fractions: Being equal or greater than one. Therefore, we present our results in Table 5.8 by running our code for a range of S from 0.1-to-5.0 to calculate the critical mass, M when f_s is about 1.0.

Table 5.8 The relation among the shape S, the Mass M and the survival fraction for the cylindrical blocks.

$N = 10^4$						
S	M	f_s		S	M	f_s
0.1	27.991	1		2.6	1.2	1.001
0.2	8.2	1		2.7	1.22	1.003
0.3	4.26	1.001		2.8	1.24	1.001
0.4	2.79	1		2.9	1.26	1.001
0.5	2.1	1		3	1.27	1.001
0.6	1.75	1.001		3.1	1.29	1.001
0.7	1.55	1.001		3.2	1.31	1.002
0.8	1.4	1.001		3.3	1.32	1.001
0.9	1.31	1.001		3.4	1.34	1.001
1	1.25	1.002		3.5	1.36	1.001
1.1	1.21	1.002		3.6	1.38	1.002
1.2	1.18	1.001		3.7	1.4	1.002
1.3	1.16	1.003		3.8	1.41	1
1.4	1.14	1.001		3.9	1.43	1
1.5	1.14	1.002		4	1.46	1.002
1.6	1.13	1.002		4.1	1.48	1.002
1.7	1.13	1.002		4.2	1.49	1.001
1.8	**1.12**	**1**		4.3	1.51	1.001
1.9	1.13	1.003		4.4	1.53	1.001
2	1.14	1.002		4.5	1.55	1.002
2.1	1.15	1.002		4.6	1.57	1
2.2	1.15	1.001		4.7	1.59	1.001
2.3	1.16	1.001		4.8	1.61	1
2.4	1.17	1.002		4.9	1.63	1.001
2.5	1.18	1.001		5	1.64	1

In order to calculate the minimum critical mass corresponding to each shape of the block (rectangular and cylinder), it required us to make the system is critical via keep the survival fraction values are equal or greater than one. In the case of the cylinder as shown in Table 5.8 we change the S value from 0.1-to-5 to calculate the *minimum critical mass* among all critical masses, we can see clearly when we change the S (shape of block) the critical mass also change. If we take a look at Table 5.8 and Figure 5.9 it shows the critical mass is decreasing and the lowest point exists when the S is equal to 1.8 (ratio of height to the radius) which give us the dimensions of the shape of the block and after 1.8 we can see the critical mass increasing until the last point of our calculation when S equal to 5.

We also present our results in Figure 5.9 to see the behavior of the mass value for a range of S where *N* is set to a constant value of N=10^4.

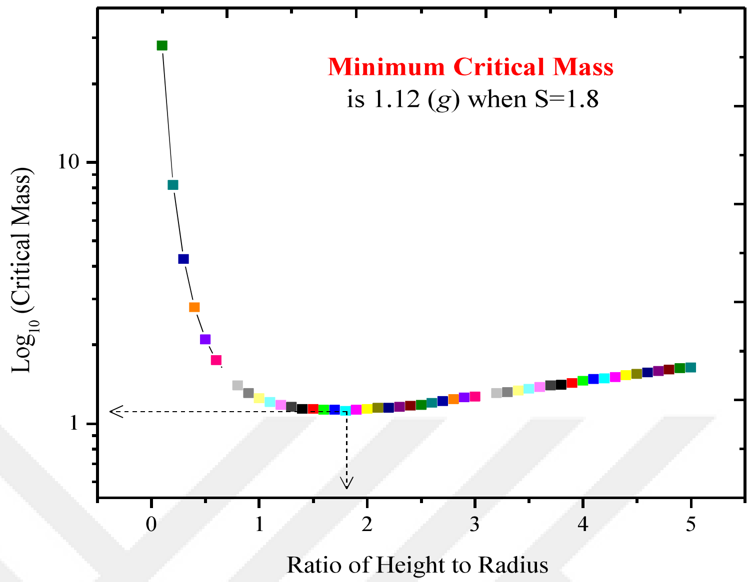


Figure 5.9 Shows the critical mass for each shape of cylindrical (It should be noted that f_s is equal or greater than 1).

The minimum critical mass is shown clearly from the Figure 5.9 when the ratio of height to the radius is equal to 1.8 ($\mathrm{S} = H/R = 1.8$). Theoretically, to calculate the minimum ratio of the height to the radius, consider a cylinder of height H and radius R, then, the volume V of the cylinder is

$$V = \pi R^2 H$$

The height to radius ratio is then

$$\mathrm{S} = \frac{H}{R} \quad \Longrightarrow \quad H = \mathrm{S}\, R$$

Hence we may write

$$V = \pi\, \mathrm{S}\, R^3 \quad \Longrightarrow \quad R = \left(\frac{V}{\pi\, \mathrm{S}}\right)^{1/3}$$

The buckling of critical reactor for a cylindrical is given by

$$B^2 = \left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2$$

Substituting $\mathrm{H} = \mathrm{S} * \mathrm{R}$ gives

$$B^2 = \left[\left(\frac{2.405}{1}\right)^2 + \left(\frac{\pi}{\mathrm{S}}\right)^2\right] * \frac{1}{R^2}$$

Then

$$B^2 = \left[\left(\frac{2.405}{1}\right)^2 + \left(\frac{\pi}{S}\right)^2\right] * \frac{S^{2/3}}{\left(\frac{V}{\pi}\right)^{2/3}}$$

$$B^2 = \left[\left(\frac{2.405}{1}\right)^2 * S^{2/3} + \left(\frac{\pi}{1}\right)^2 S^{-2} * S^{2/3}\right] * \frac{1}{\left(\frac{V}{\pi}\right)^{2/3}}$$

$$B^2 = \left[(2.405)^2 * S^{2/3} + (\pi)^2 * S^{-4/3}\right] * \left(\frac{\pi}{V}\right)^{2/3}$$

For the minimum buckling with constant V, we have to derivative with respect to S

$$\frac{d}{ds}B^2 = 0$$

$$\frac{d}{ds}B^2 = \frac{d}{ds}\left\{\left[(2.405)^2 * S^{2/3} + (\pi)^2 * S^{-4/3}\right] * \left(\frac{\pi}{V}\right)^{2/3}\right\}$$

$$\frac{d}{ds}B^2 = \left(\frac{\pi}{V}\right)^{2/3} * \left[(2.405)^2 * (2/3) * S^{-1/3} + (\pi)^2 * (-4/3) * S^{-7/3}\right] = 0$$

$$(2.405)^2 * (2/3) * S^{-1/3} - (\pi)^2 * (4/3) * S^{-7/3} = 0$$

$$\frac{-13.15947 + 3.856016667 * S^2}{S^{7/3}} = 0$$

The result is found to be

$$S \cong 1.8$$

5.4 Calculation of the Critical Mass for a Bare Spherical Reactor

Spherical coordinates, that are also called as spherical polar coordinates ($Walton -$ 1967, $Arfken$ 1985), are a system of curvilinear coordinates that are natural for describing positions on a sphere or spheroid. Define ϕ to be the azimuthal angle in the xy-plane from the x-axis with $0 \leq \phi < 2\pi$ (denoted λ when referred to as the longitude), θ to be the polar angle (also known as the zenith angle and colatitude, with $\theta = 90^{\circ} - \delta$ where δ is the latitude) from the positive z-axis with $0 \leq \theta \leq \pi$, and r to be distance (radius) from a point to the origin. This is the convention commonly used in mathematics [13].

We calculate the critical mass of spherical shape which just depends on the radius 'R' [38]. To determine the critical mass for a spherical shape there is a direct relationship between the mass and the radius and based on the eq. (5.7) it can be changing each other directly. Therefore, under the condition the density is constant, it cannot keep the radius (r) fixed and vary the mass of the block (M); here we must changing the mass until the *survival fraction* f_s has the value 1.0.

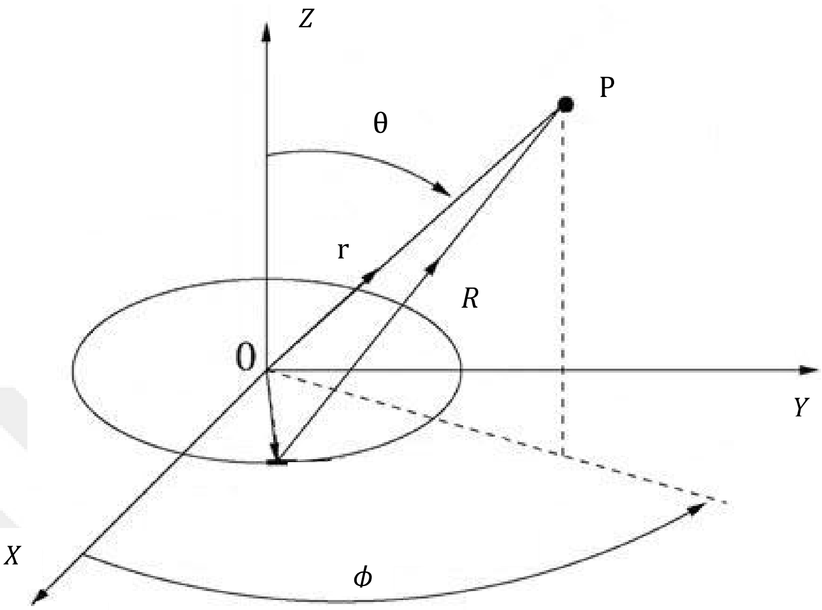


Figure 5.10 Spherical coordinates systems.

The dimensions of r can easily be found in terms of M.

$$\mathrm{r} = \left(\frac{3\ \mathrm{M}}{4 * \pi}\right)^{1/3} \tag{5.7}$$

The Cartesian coordinates $(\mathrm{x}, \mathrm{y}, \mathrm{z})$ are related to the spherical coordinates by

$$\begin{aligned} \mathrm{x}_0 &= \mathrm{r}\ \cos\theta\ \sin\phi \\ \mathrm{y}_0 &= \mathrm{r}\ \sin\theta\ \sin\phi \\ \mathrm{z}_0 &= \mathrm{r}\ \cos\phi \end{aligned} \tag{5.8}$$

where $\mathrm{r} \in [0, \infty), \phi \in [0,2\pi)$ and $\theta \in [0, \pi)$. We assumed that all fissions occurred inside the boundary conditions:

$$\begin{aligned} -\mathrm{r} &< \mathrm{x}_0 < \mathrm{r} \\ -\mathrm{r} &< \mathrm{y}_0 < \mathrm{r} \\ -\mathrm{r} &< \mathrm{z}_0 < \mathrm{r} \end{aligned} \tag{5.9}$$

where $\mathrm{x}_0, \mathrm{y}_0$, and z_0 are coordinates of the fission which emitting a neutron inside the boundaries of the reactors.

By running the program using a range of values for the number of randomly generated neutrons *N*, we present our results in Tables 5.9 and 5.10.

Table 5.9 Shows the relation between the number of initial neutrons *N* and the survival fraction for the spherical.

1st set ($M = 1 \implies r = 0.62035$)						
N	10^2	10^3	10^4	10^5	10^6	10^7
f_s	1.11	1.081	1.0765	1.08025	1.079055	1.0795062
	1.05	1.094	1.0829	1.07873	1.078407	1.0795276
	1.08	1.075	1.0975	1.08197	1.080221	1.0798335
	0.98	1.072	1.0697	1.07738	1.079912	1.0796746
	1.01	1.074	1.0773	1.07759	1.080022	1.0797197
	1.23	1.088	1.0906	1.07516	1.078738	1.0797584
	1.02	1.098	1.0706	1.07756	1.079784	1.0798805
	0.99	1.113	1.0888	1.08207	1.079915	1.0799033
	1.12	1.097	1.0835	1.07789	1.079364	1.0797344
	0.89	1.071	1.083	1.08052	1.079512	1.0799324
$\bar{f_s}$	1.048	1.0863	1.08204	1.078912	1.079493	1.07974706
$T(s.)$	0.1404	1.1388	11.0916	108.79	1139.322	11132.77

As seen in Table 5.9, the range of the number of neutrons (*N*) for six cases are $(10^2, 10^3, \dots, 10^7)$ where it can be observed that the accuracy of the survival fraction depends on the number of neutrons and in order to be outcomes of the survival fraction more accurate it had to be increased the number of neutrons. We can make the system be critical via increasing the mass of the block M. By running the program, we can let $N = 10^6$ for all runs, and then the outcomes are given in Table 5.10.

Table 5.10 Shows the relation between the mass M and the survival fraction for the cylindrical blocks.

	2nd set ($N = 10^6$ and r Proportional to M)						
M	0.1	0.5	1.0	1.5	2	8	16
f_s	0.50245	0.85972	1.079055	1.22369	1.32693	1.71484	1.81662
	0.502304	0.858557	1.078407	1.22491	1.32702	1.71549	1.81686
	0.501367	0.859933	1.080221	1.22434	1.32843	1.7141	1.81761
	0.502028	0.859054	1.079912	1.22486	1.32756	1.71526	1.81713
	0.502472	0.85819	1.080022	1.22377	1.32732	1.71596	1.81684
	0.502949	0.859321	1.078738	1.22291	1.32857	1.71641	1.8178
	0.502682	0.858887	1.079784	1.22511	1.32756	1.71544	1.81753
	0.501119	0.859023	1.079915	1.22361	1.32772	1.71567	1.81654
	0.502602	0.858892	1.079364	1.22317	1.32825	1.71583	1.81748
	0.502316	0.860172	1.079512	1.2242	1.32706	1.71533	1.81679
$\bar{f_s}$	0.502229	0.859175	1.079493	1.22406	1.32764	1.71543	1.81712
$T(s.)$	1113.23	1119.088	1139.322	1108.02	1131.70	1087.139	1130.91

The effect of the increasing the mass is shown clearly by increasing its value, the critical mass appeared at M=1 but does not mean minimum critical mass because there is a big gap from 0.5 to 1 and it can make the system is critical in case of the mass less than 1. The Figure 5.11 gives us a clearer idea of this effect.

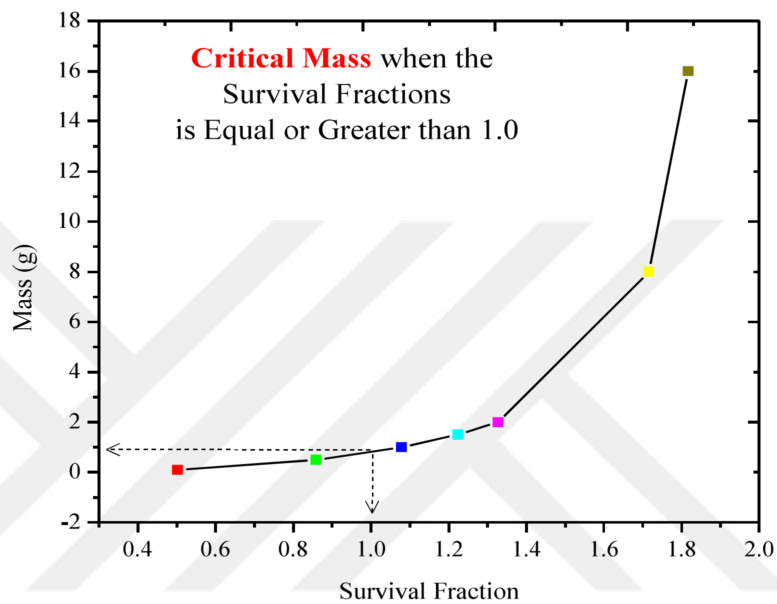


Figure 5.11 Shows the effect of mass M of the block on the survival fraction for the spherical blocks.

We use the range of the masses to find the corresponding critically conditions for the mass and the critical mass appears when the survival fraction is equal or greater than one. With a view to seeing the effect of changing the shape clearly has been drawn in Figure 5.12. As it is mentioned earlier in Chapter 3; when one writes the steady state diffusion equation, the production and absorption of neutrons are proportional to the core volume and the volume of the sphere is $V = (4/3)\,\pi\, \mathrm{r}^3$ where the neutrons' leakage are proportional to the core surface for which one has $A_S = 4\,\pi\, \mathrm{r}^2$. Therefore, the number of neutrons lost (by leakage) from the core surface of reactor could be decreased when the core surface is increased. In summary, the decrease in number of leakage neutrons via increasing the size of core will subsequently lead to the increase in the value of survival fraction.

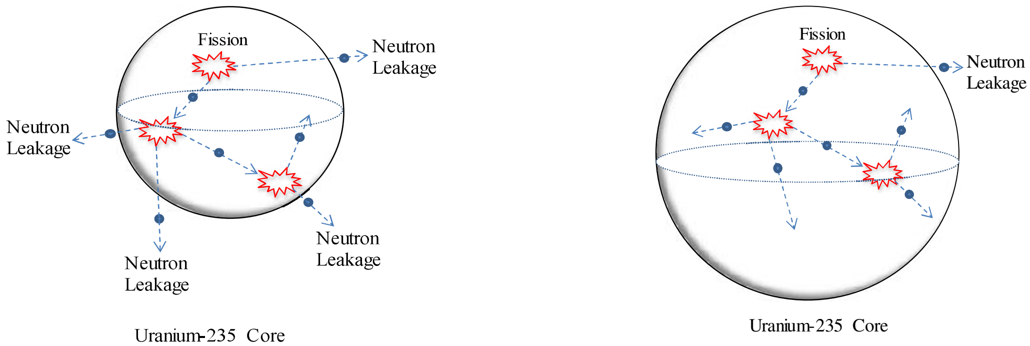


Figure 5.12 Shows the virtual fission processes inside the spherical coordinates systems.

To know what the minimum critical mass and the supercritical mass are for the certain values of the radius from (0.133 *cm* to 1.054 *cm*), it required us to running the program until making the system critically through the survival fractions when to be equal or greater than one. Where it had been calculated the critical mass for each radius as shown in Table 5.11.

Table 5.11 The relation among the radius r, the Mass M and the survival fraction for the spherical blocks for $N = 10^4$.

$N = 10^4$						
M	r	f_s		S	r	f_s
0.01	0.13365046175719	0.232794		2.51	0.8430662505402691	1.40785
0.11	0.29723596604340	0.518616		2.61	0.8541168689614519	1.42043
0.21	0.36873149012643	0.641612		2.71	0.8648887084004276	1.43242
0.31	0.41984697474723	0.731956		2.81	0.8753987124977887	1.44579
0.41	0.46085582641628	0.802502		2.91	0.8856622349651657	1.4569
0.51	0.49563335105656	0.8655		3.01	0.8956932377779163	1.46772
0.61	0.52611466622751	0.917306		3.11	0.9055044589543568	1.47775
0.71	0.55342220426276	0.963154		3.21	0.915107555408887	1.48938
0.81	**0.57827196312211**	**1.00713**		3.31	0.9245132252374069	1.49851
0.91	0.60115195111789	1.04645		3.41	0.9337313129236117	1.50809
1.01	0.62241147112564	1.08239		3.51	0.9427709002787857	1.5174
1.11	0.64231015723657	1.11556		3.61	0.9516403853981289	1.52693
1.21	0.66104687068166	1.14656		3.71	0.9603475514986	1.53269
1.31	0.67877769404322	1.17606		3.81	0.9688996271708928	1.54129
1.41	0.69562764730936	1.20057		3.91	0.9773033393121482	1.54837
1.51	0.71169860188010	1.22655		4.01	0.9855649597917352	1.5577
1.61	0.72707479398209	1.24903		4.11	0.993690346728835	1.56304
1.71	0.74182676808703	1.27203		4.21	1.0016849811190902	1.57081
1.81	0.75601426217138	1.29276		4.31	1.009553999431691	1.57512
1.91	0.76968836096245	1.30972		4.41	1.0173022227028519	1.58301
2.01	0.78289313111987	1.33061		4.51	1.0249341825726785	1.58908

for Table 5.12 to be more understandable, it may be transferred the data in the form of a drawing as shown in Figure 5.13.

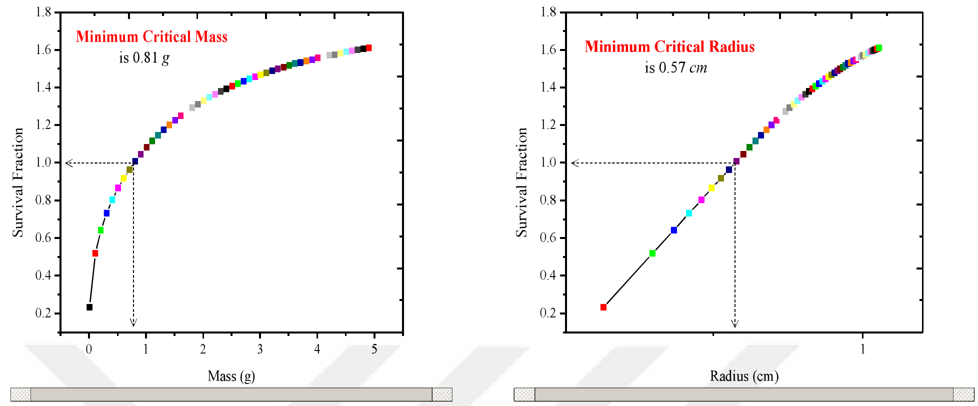


Figure 5.13 Shows the critical mass corresponding to each radius of sphere (It should be noted that f_s is equal or greater than 1).

The minimum critical mass with proportion to the minimum radius as explained in Eq. (5.7) and it has been drawn for both of them; the first gives us the survival fraction in respect to each mass and in this point, there is a corresponding radius as we drawn it in the second figure where the minimum critical mass is 0.81 g appears when the radius is 0.57 cm and after this point, we can say the system has become critical because the survival fraction is greater than one.

The system can be built to be critical in a number of shapes: In case the self-sustaining chain reacting system is to be built in the form of a large spherical structure, the critical radius is then given by

$$B^2 = \left(\frac{\pi}{\mathrm{r}}\right)^2$$

In case the structure is to be a rectangular parallelepiped with side a, b and c, the critical size is given by the formula

$$B^2 = \left(\frac{\pi}{a} + \frac{\pi}{b} + \frac{\pi}{c}\right)^2$$

In case the structure is to be built up as a cylinder of height H and radius R, the critical values of these quantities may be computed from the formula

$$B^2 = \left(\frac{\pi}{H^2} + \frac{2.405}{R^2}\right)^2$$

When one is talking about the critical dimensions, it must be linked to the critical mass of fuel used because the critical mass of fuel for any shape of geometry through these dimensions can be minimized. We determine the relationship between the buckling and the dimensions of the geometries when the size of the reactor is such that the chain reaction is kept constant for which we refer as critical size. In our study, we find that the sphere has the smallest critical size, while the rectangular one has the largest. Since the spherical geometries are very difficult to construct in practice, most reactors therefore are built in shape of cylindrical form. The prior results can now be the comparison of determining the critical components or critical dimensions of a bare fast reactor. It can be seen that for a given amount of material in the system, the spherical shape is to be the one preferred for minimum mass, and the Table 5.12 shows the summary for the comparison among three geometries as we present our numerical results throughout the Chapter [39-42].

Table 5.12 Reactor geometries, volume, corresponding bucklings and critical mass.

Core Shapes	Buckling (B)		Critically Relation	Critical Dimensions
	Material-B	Geometric-B		
Rectangular parallelepiped	$B^2 = \frac{k_\infty - 1}{L^2}$	$B^2 = \left(\frac{\pi}{a} + \frac{\pi}{b} + \frac{\pi}{c}\right)^2$	$V_c = \frac{161.11}{B^3}$	$a = b = c$ (cubic shape)
Finite Cylinder	$B^2 = \frac{k_\infty - 1}{L^2}$	$B^2 = \left(\frac{\pi}{H} + \frac{2.405}{R}\right)^2$	$V_c = \frac{148.00}{B^3}$	$R = 0.58$ $H = 1.04$
Sphere	$B^2 = \frac{k_\infty - 1}{L^2}$	$B^2 = \left(\frac{\pi}{\mathrm{r}}\right)^2$	$V_c = \frac{126.63}{B^3}$	r = 0.57

CHAPTER 6

CONCLUSION

In this thesis, we focus on the coding of a computer program by using *Wolfram™ Mathematica© 9* to study and simulate the fission chain reaction for fissile elements, such as uranium, by the Monte Carlo Method (MCM). The critical mass for a rectangular block, cylindrical shape of source and finally a spherical piece of fissile material is firstly determined by the solution of the steady-state one group diffusion equation for the geometric and material buckling parameters. Then, the main definitions and parameters for a simulation of the fission process are introduced, in details, to calculate the survival fraction for a range of masses and shapes mentioned throughout the chapter. The code is based on the generation of random numbers for certain set of parameters such as the induced fission position, the mean free path for each generated neutron, the position of new fission point after the motion of new neutrons through the mean free path, etc.

In this study, we write and run our code for three different geometries. In case of a bare rectangular parallelepiped, we find that the minimum critical mass exists when the ratio of length-to-thickness ($\mathrm{S} = a/b$) is equal to 1. At this point one can say the minimum critical size takes place if it is in the shape of a cube. In the case of a bare finite cylinder we determine that the minimum critical mass occurs when the ratio height-to-radius ($S = H/R$) is equal 1.8 which gives us the dimensions of the shape. For the bare sphere, the minimum critical mass exists when the radius of the sphere is equal 0.57 *cm* for our hypothetical shape. It is clear that our numerical results are not dimensions of real systems. We obviously obtain and show the solutions of the one-group steady-state diffusion equation for the buckling parameter using the MCM code written by us for the simplest case to determine the minimum critical mass case.

We compare our MCM outputs with diffusion theory equations for Zero Boundary Flux case and it is important to point out here that our results are exactly in agreement with theoretical ones of the Diffusion Theory. As it is shown throughout the results, the most optimum shape among all three geometries from the view point of minimum fissile mass requirements for reaching the minimum critical mass case is the spherical shape system.

Since our calculations based on the Diffusion Theory with Zero Boundary Flux case, one can study the case for the Extrapolated Boundary Flux for the neutron flux in other geometries with the certain amount of material mixture for the fuel element as a future study. The code can be modified for more realistic systems by taking into consideration the rest of the influencing parameters such as energy of neutrons and corresponding cross-section values of target element and etc. There is also possibility to calculate the critical mass in simple reactor geometries with reflectors which are good at reducing the amount of fuel that is required for a core to become critical. Therefore, adding a reflector to any of these geometries can be studied in the light of this thesis and the results presented throughout the text. Finally, there is also possibility to modify our code to calculate the critical mass for other particular geometries and compare the results among them.

REFERENCES

[1] A. Das and T. Ferbel, *Introduction to nuclear and particle physics*, 2nd ed. New Jersey: World Scientific, 2003.

[2] K. S. Krane, *Introductory Nuclear Physics*, Rev. New York: John Wiley & Sons, Inc., 1988.

[3] Y. A. Cengel and M. A. Boles, *Thermodynamics: an Engineering Approach 8th Edition*. 2015.

[4] J. R. Lamarsh and A. J. Baratta, *Introduction to Nuclear Engineering*, 3rd ed. United States of America: Prentice-Hall, 2001.

[5] W. M. Stacey, *Nuclear Reactor Physics*, 2nd ed. United States of America: Wiley-VCH Verlag GmbH & Co. KGaA, 2007.

[6] E. E. Lewis, *Fundamentals of Nuclear Reactor Physics*, 1st ed. Amsterdam [etc.]: Academic Press, 2008.

[7] D. Kastanya, "Critical mass calculations using MCNP: An academic exercise," *Ann. Nucl. Energy*, **75**, pp. 228–231, 2015.

[8] E. Brandon, "A Monte Carlo Approach to the Calculation of the Critical Mass," *Michigan State Univ.* **PHY**, p. 492, 2015.

[9] A. Idris, Y. Y. Ibrahim, and M. Auwal, "Investigation of General Equation That Best Describe the Relationship between Survival Fraction and Critical Mass of Uranium (235)," *J. Appl. Phys.*, **7(1)**, pp. 06–10, 2015.

[10] A. Idris and Y. Y. Ibrahim, "Determination of Minimum Critical Mass of U235 Using Monte Carlo Method," *Niger. Assoc. Math. Phys.*, **23**, pp. 255 – 264, 2013.

[11] A. W. Gray, "Minimum Critical Mass of Uranium-235 Reflected by Natural

Uranium in Water," *Nucl. Technol.*, **12(4)**, pp. 342–347, 1971.

[12] O. Hiroshi and K. Hiromitsu, "Critical and Subcritical Mass Calculations of Curium-243 to -247 Based on JENDL-3.2 for Revision of ANSI/ANS-8.15," *J. Nucl. Sci. Technol.*, **39(10)**, pp. 1072–1085, 2002.

[13] E. W. Weisstein, "Spherical Coordinates," *http://mathworld.wolfram.com/SphericalCoordinates.html*. Wolfram Research, Inc., 2005.

[14] D. G. Madland, "Total prompt energy release in the neutron-induced fission of 235U, 238U, and 239Pu," *Nucl. Phys. A*, **772(3–4)**, pp. 113–137, 2006.

[15] J. R. Lamarsh, *Introduction to Nuclear Reactor Theory*, 1st ed. New York: Addison-Wesley Publishing Company, 1966.

[16] B. Viswanathan, *Energy sources: fundamentals of chemical conversion processes and applications*, 1st ed. Cheenai, india: Newnes, 2016.

[17] G. Friedlander, J. M. Miller, E. S. Macias, and J. W. Kennedy, *Nuclear and radiochemistry*, 3rd ed. New York: John Wiley & Sons, 1981.

[18] K. Nishio, Y. Nakagome, I. Kanno, and I. Kimura, "Measurement of fragment mass dependent kinetic energy and neutron multiplicity for thermal neutron induced fission of plutonium-239," *J. Nucl. Sci. Technol.*, **32(5)**, pp. 404–414, 1995.

[19] G. Espinosa-Paredes, M. A. Polo-Labarrios, and J. Alvarez-Ramirez, "Anomalous diffusion processes in nuclear reactors," *Ann. Nucl. Energy*, **54**, pp. 227–232, Apr. 2013.

[20] S. Dababneh, K. Khasawneh, and Z. Odibat, "An alternative solution of the neutron diffusion equation in cylindrical symmetry," *Ann. Nucl. Energy*, **38(5)**, pp. 1140–1143, 2011.

[21] B. C. Reed, "Note on the minimum critical mass for a tamped fission bomb core," *Am. J. Phys.*, **83(11)**, pp. 969–971, 2015.

[22] R. Vázquez-Rodríguez, G. Espinosa-Paredes, J. B. Morales-Sandoval, A.

Vázquez-Rodríguez, and E.-G. Espinosa-Martinez, "Averaging the neutron diffusion equation," *Prog. Nucl. Energy*, **51(3)**, pp. 474–484, Apr. 2009.

[23] K. Khasawneh, S. Dababneh, and Z. Odibat, "A solution of the neutron diffusion equation in hemispherical symmetry using the homotopy perturbation method," *Ann. Nucl. Energy*, **36(11–12)**, pp. 1711–1717, 2009.

[24] C. Jacoboni and L. Reggiani, "The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials[J]," *Rev. Mod. Phys.*, **55(3)**, pp. 645–705, 1983.

[25] D. P. Landau, S.-H. Tsai, and M. Exler, "A new approach to Monte Carlo simulations in statistical physics: Wang-Landau sampling," *Am. J. Phys.*, **72(10)**, pp. 1294–1302, 2004.

[26] N. Metropolis and S. Ulam, "The Monte Carlo Method," *J. Am. Stat. Assoc.*, **44(247)**, pp. 335–341, 1949.

[27] F. James, "Monte Carlo theory and practice," *Reports on Progress in Physics*, **43(9)**. pp. 1145–1189, 1980.

[28] T. Kristóf and G. Rutkai, "Dynamic Monte Carlo simulation in mixtures," *J. Chem. Phys.*, **132(10)**, 2010.

[29] A. M. Ferrenberg, D. P. Landau, and Y. J. Wong, "Monte Carlo simulations: Hidden errors from good random number generators," *Phys. Rev. Lett.*, **69(23)**, pp. 3382–3384, 1992.

[30] B. Lennart, B. Jonathan M, and B. Peter B, *Pi: A Source Book*, 3rd ed. New York: Springer, 2004.

[31] A. M. Ferrenberg, D. P. Landau, and Y. J. Wong, "Monte Carlo simulations: Hidden errors from '"good"' random number generators," *Phys. Rev. Lett.*, **69(23)**, pp. 3382–3384, Dec. 1992.

[32] A. N. Borodin, *Stochastic Processes*. Cham: Springer International Publishing, 2017.

[33] H. VAN DAM and D. L. P. F. A., “MINIMUM CRITICAL MASS SYSTEMS,” *Ann. Nucl. Energy*, **14(7)**, pp. 369–376, 1987.

[34] J. Bernstein, “Heisenberg and the critical mass,” *Am. J. Phys.*, **70(9)**, pp. 911–916, 2002.

[35] B. C. Hacker, *The dragon’s tail: radiation safety in the Manhattan Project*. Univ of California Press, 1987.

[36] T. Jacobsen and K. West, “Diffusion impedance in planar, cylindrical and spherical symmetry,” *Electrochim. Acta*, **40(2)**, pp. 255–262, 1995.

[37] E. W. Weisstein, “Cylindrical Coordinates,” *http://mathworld.wolfram.com/CylindricalCoordinates.html*. Wolfram Research, Inc., 2005.

[38] J. S. Cassell and M. M. R. Williams, “A solution of the neutron diffusion equation for a hemisphere with mixed boundary conditions,” *Ann. Nucl. Energy*, **31(17)**, pp. 1987–2004, 2004.

[39] J. Kemsley, “Determining nuclear weapons yields from bomb debris,” Chem. & Eng. News, **94(28)** pp. 9-9, 2016.

[40] B. C. Reed, “The Manhattan Project,” Physica Scripta, **89(10)**, 2014.

[41] P. Signell, “Poject Physnet,” www.physnet.com. 2002.

[42] R. Q. Wright and C. M. Hopper, “Calculation of the minimum critical mass of fissile nuclides,” Nucl Sci. Eng., **158(2)**, pp. 203-209, 2008.