Calculation of the Critical Mass

and

the Eigenvalue of Fast Neutrons Reaction

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Engineering Physics University of Gaziantep

Supervisor Assoc. Prof. Dr. Okan ÖZER

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ABSTRACT

CALCULATION OF THE CRITICAL MASS AND THE EIGENVALUE OF FAST NEUTRONS REACTION

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Solution of the steady-state one-group diffusion equation for bare and reflected reactors in three distinct geometries has great importance in the calculation of the critic size and critical mass of the pure or mixtured fuel material. The eigenvalue of the diffusion equation shows the relation between the material and the size of the geometry in question. This relation is called the material Buckling, B_m , or the geometric Buckling, B_g . Solving the steady-state one-group diffusion equation for bare reactor systems, the critical mass values are obtained in three distinct geometries for different material structures. After surrounding a bare reactor with a reflector material, a reduction is observed in the critic dimensions in all geometries and also the critical mass decreases to a certain value depending on the properties of the reflector thickness. The results obtained in this study are compared with the numerical values existing in the literature.

Key words: critic mass, diffusion equation, fast neutrons

ÖZET

KRİTİK KÜTLE VE HIZLI NÖTRONLARIN REAKSİYONLARININ ÖZ DEĞER HESAPLAMALARI

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Üç farklı geometrideki yalın ve reflektörlü reaktörlerin kararlı hal tek grup difüzyon denklem çözümleri saf ve karışımlı yakıt malzemeli kritik kütle hesapları tartışmaları büyük bir öneme sahiptir. Difüzyon denkleminin öz değeri reaktörün gerekli olan minimum boyut ve malzeme ilişkisini verir. Bu ilişki malzeme B_m ve geometri bükülme B_g olarak adlandırılır. Öncelikle kararlı hal tek grup difüzyon denklemi çözülerek üç farklı geometrili (küre, silindir ve dikdörtgen prizma) yalın reaktörlerin kritik kütle değerleri farklı materyal yapıları için elde edildi. Yalın reaktör reflektörle kaplandıktan sonra, bütün geometrideki reaktörlerin kritik boyutlarında küçülme gözlenmiştir. Ayrıca kritik kütle de reflektörün ve yakıt malzemesinin özelliğine bağlı olarak belli bir değere kadar düşmektedir. Bu çalışmadaki hesaplama sonuçları literatürdeki sayısal sonuçlarla karşılaştırılmıştır.

Anahtar kelimeler: kritik kütle, difüzyon denklemi, hızlı nötronlar

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CONTENTS

ABSTRACTiv
ÖZETv
ACKNOWLEDGEMENTSvi
CONTENTS
LIST OF FIGURESix
LIST OF TABLESx
LIST OF SYMBOLSxi
CHAPTER 1:GENERAL INTRODUCTION1
CHAPTER 2: THEORITICAL INFORMATION
2.1 INTERACTION OF NEUTRONS WITH MATTER
2.1.1 THE PRODUCTION OF NEUTRONS
2.1.2 NEUTRON ABSORPTION REACTIONS
2.1.2.A Radiative Capture Reactions7
2.1.2.B Charged Particle Emission
2.1.2.C Fission Reactions
2.1.3 NEUTRON SCATTERING REACTIONS10
2.1.3.A Elastic Scattering11
2.1.3.B Inelastic Scattering
2.2 CROSS-SECTIONS and NEUTRON FLUX
2.2.1 Microscopic Reaction Cross-Sections
2.2.2 Macroscopic Reaction Cross-Sections17
2.2.3 Neutron Flux
2.2.4 FICK'S LAW
CHAPTER 3: SOLUTION OF DIFFUSION EQUATION FOR NON-
MULTIPLYING SYSTEMS
3.1 EQUATION OF CONTINUITY
3.2 THE DIFFUSION EQUATION

3.3 SOLUTION OF THE DIFFUSION EQUATION IN NON-MULTIPLYIN SYSTEMS	IG 39
3.3.1 Infinite planer source	39
3.3.2 Point source	42
3.3.3 Bare slab	43
3.3.4 Two region example for sphere with source	46
CHAPTER 4: SOLUTION OF DIFFUSION EQUATION FOR MULTIPLYIN SYSTEMS	IG 50
4.1 SUBCRITICAL ASSEMBLIES FOR SPHERE	50
4.1.1 Subcritical assemblies for sphere	51
4.1.2 Supercritical assemblies for sphere	53
4.2 CRITICAL ASSEMBLIES FOR DIFFERENT GEOMETRIES	55
4.2.1 The slab reactor	55
4.2.2 Sphere	58
4.2.3 Infinite Cylinder	63
4.2.4 Finite cylinder	67
4.2.5 Rectangular parallel piped	75
CHAPTER 5: REFLECTED REACTORS	79
5.1 Axial reflector	79
5.2 Spherical reflector	84
CHAPTER 6: CONCLUSION	90
REFERENCES	92
APPENDIX	94

LIST OF FIGURES

PAGE

Figure 2.1 Schematics of the potential elastic neutron scattering11
Figure 2.2 Geometry for neutron reaction rate in thin target of volume V14
Figure 2.3 Geometry for the derivation of the neutron current and Fick's Law24
Figure 2.4 Neutron flux and current
Figure 2.5 Neutron flux and current in the wall of reactor
Figure 3.1 Extrapolation distance
Figure 3.2 Planer source at origin x=0
Figure 3.3 Infinite slab with planar source at x=044
Figure 4.1 Slab reactor
Figure 4.2 Ordinary and modified Bessel functions
Figure 5.1 Axial - Reflector80
Figure 5.2 Calculated reflector saving as a function of Uranium reflector thickness 88
Figure B.1 Extrapolation distance of neutron flux at plane surface between diffusion medium and vacuum

LIST OF TABLES

Table 2.1 Cross section symbols for different type of reaction
Table 4.1 Neutron cross-sections for ²³⁵ Uand ²³⁹ Pu used in Ref. [16].
Table 4.2 The critic radius and critic mass values at 2MeV neutron cross-sections for ²³⁵ U from data library [ENDF/B-VII.1]
Table 4.3 Critical radius for infinite cylinder
Table 4.4 Comparison of chosen heights and the corresponding critical radii with extrapolated distance and non-extrapolated distance for bare finite cylinder of 235U.
Table 4.5 Chosen heights and the corresponding critical radii and critical masses with extrapolated distance and non-extrapolated distance for ²³⁵ U, for 2MeV neutrons73
Table 4.6 Chosen heights and the corresponding critical radii and critical masses withextrapolated distance and non-extrapolated distance for ²³⁹ Pu, for 2MeVneutrons
Table 4.7 Buckling and flux distributions in Bare systems for distinct geometries78
Table 5.1 Axial Uranium core and Uranium reflector 83
Table 5.2 Axial Uranium core- Pu-239 Reflector.84
Table 5.3 Pure ²³⁵ U core surrounded with pure ²³⁵ U reflector for sphere
Table 5.4 Pure ²³⁹ Pu core surrounded with pure ²³⁹ Pu reflector for sphere. 89
Table 5.5 Comparision of spherical reflector results with literature 89

LIST OF SYMBOLS

ϕ	Neutron Flux Function
d	Extrapolation Distance
<i>˜R</i>	Extrapolated Radius of a Sphere
R_c	Critic Radius of a Sphere
δ	Reflector Savings
σ	Microscopic Cross Section
Σ	Macroscopic Cross Section
k	Multiplication Factor
k_{∞}	Multiplication Factor for Infinite Medium
$\overrightarrow{\nabla}$	Gradient Operator
∇^2	Laplacian Operator
L	Diffusion Length
$D_{c,r}$	Diffusion Coefficient (for core and reflector, respectively)
$ec{J}$	Neutron Current Density Vector
λ_{tr}	Transport Mean Free Path
В	Buckling
B_g	Geometrical Buckling
B_m	Material Buckling

CHAPTER 1

GENERAL INTRODUCTION

Nuclear power plants are substantially efficient in energy production and still being used by lots of countries all over the world. With thriving technology, nuclear power reactor types are multiplied by time. Although the reactor types are different, the basic components of these systems are the same. A nuclear reactor is basically composed of several elements like moderator, coolant, control rods, blanket and reflector. The moderator is used to slow down the neutrons from fission to thermal energy levels. The coolant is used to remove the heat from the core and the other parts of the reactor. The blanket is the part of the reactor made of fertile material that surrounds the core of the breeder reactors. As understandable, control rods are movable pieces of neutron-absorbing material which are used to control the criticality of the reactor. Lastly, the reflector is adjacent to the core that catches the neutrons escaping after more collisions from the core of reactor. This study also includes reflector saving calculations.

The heart of a fission reactor, the fission takes place in the core, breeds the whole power plant with fission chain reaction energy. Accordingly Uranium and its isotopes are essential for a fission reactor that produces energy from fission reactions. The natural uranium consists of 99.27 % of Uranium-238, 0.72 % of Uranium-235 and 0.0057 % of Uranium-234. [1, 2]. Uranium-235 is more effective in fission by thermal neutrons and also more preferable in practice because of some certain reasons such as Binding energy and the activation energy of Uranium isotopes. Due to limited amount of Uranium-235, enrichment and various compositions are used in core for fission chain reaction as an energy source. Furthermore, importance of critic mass appears due to the little amount of Uranium-235 isotope in natural uranium. Critic mass is the smallest mass for sustaining the

fission chain reaction in a nuclear power reactor. The denoted parameter k, called as "multiplication factor" (or survival factor) is the ratio of the number of neutrons generated in present fission to the number of neutrons generated in the previous fission [3]. Therefore, the parameter k can get three different values: If k is less than 1, then the number of fission chain reactions decrease with time and the energy production reduces in time. This condition is called "subcritical". If k is equal to 1, then the generation of fission neutrons is stable and the reactor is called "critical". If k is greater 1, then the generation of neutrons increase with time and the reactor is called "supercritical". As a result of these conditions, the generation of fission neutrons gets great importance in the reactor core which may be made of different composition of uranium isotopes.

In the reactor core that has fissionable material there occur many kinds of neutron interactions like elastic- inelastic scattering of neutrons and radiative capture reaction as well as fission reaction. These interactions fluctuate the number of neutrons in the core composition. Some interactions increase, others decrease the neutron population with time. So, the flux and also the density calculations require obtaining the net number of neutrons at the boundaries of the core. To determine the neutron flux in the reactor core, neutrons may be assumed to be solute in a solution: The density goes from region of high concentration to that of low concentration region. As a good approximation, Fick's Law [4] for neutron diffusion in reactor core can be used. Furthermore, Fick's Law states that the rate of solute flow is proportional to the negative of the gradient of the solute concentration [1, 3]. So, Fick's law is the starting point for the solution of diffusion equation in the determination of the parameters required to calculate the multiplication factor (or survival factor), k. Then calculations are done for the reveal the critic mass of reactor core.

The most general form of the diffusion equation for fission neutrons depends on geometry of the system and the time variable. If one does not consider the reactor kinetics for time parameter, then an important question arises: For what geometry the critical mass is the lowest one? To answer this curious question, initially the most primitive system that is one-group (fast-group because of narrow energy range than thermal group) steady-state neutron diffusion equation is considered. In this thesis, the solution of the one-group steady-state neutron diffusion equation for certain distinct geometries is obtained and the critical mass calculations are studied.

In Chapter 2, the neutron interactions with matter and the derivation of the Fick's law is given. Definitions of the microscopic and macroscopic cross-sections, neutron flux, mean-free path are discussed.

In Chapter 3, the equation of continuity is obtained and the solution of the steadystate neutron diffusion equation for non-multiplying media is considered. Solutions are obtained for certain reactor geometries: Solutions of the diffusion equation are done to understand the behavior of neutron flux for non-multiplying systems consisting of a point source, an infinite planer source and a bare slab. These calculations help to understand the solution of non-multiplying bare systems.

A bare reactor is considered with multiplying medium that consists of fissionable materials in Chapter 4. The diffusion equation with multiplying media has an eigenvalue which is called the *material buckling* related with the composition of the core material. Here, the term "buckling" is defined by the curvature or bending of the neutron flux in the system. The analytical or numerical expression of the buckling parameters for different specific reactor systems is determined by expressing the Laplacian operator in the most appropriate coordinates that depend on the reactor shape and then one can solve the resultant steady-state differential equation subject to the boundary conditions of the system under investigation. In general, the expression of the buckling parameter satisfying the mathematical requirements of the differential equation is not unique but the smallest numerical value has physical significance in the solution of the problem. It is shown in this Chapter why one shall be interested in obtaining the smallest value of the buckling parameter.

Surrounding a bare system with a reflector, that is a medium having high scattering cross section and low absorption cross section, has some certain advantages which are studied in Chapter 5. Since the power production in the reactor core is also proportional to the average neutron flux in the system, the reactor can be run at a higher total power output for the same neutron flux if it is maximized throughout the system. The effect of flux-flattening is observed as the higher power production rate especially in large power reactors from the operational point of view. If one can obtain the neutron flux function for the geometry in the question, then the power produced in this system can also be calculated by using the type of fissile material and its fission energy value. However, the main purpose of this thesis study focuses on the critic size and mass of the reactor core. After determining the critical mass value for the bare systems in certain geometries, the calculations are done for the same systems with certain type of reflector materials. Our results are compared with the existing literature.

CHAPTER 2

THEORITICAL INFORMATION

2.1 INTERACTION OF NEUTRONS WITH MATTER

In this Chapter a brief information about the neutron interactions is given.

2.1.1 The Production of Neutrons

Neutron sources are various kinds of required for experimental purpose and also play an important role in the start-up of nuclear reactors. Neutrons are obtained by the action of alpha particle on some light elements like beryllium, boron, or lithium. The reaction [5] may be shown by

$${}^{9}_{4}Be + {}^{4}_{2}He \longrightarrow {}^{12}_{6}C + {}^{1}_{0}n$$
(2.1)

Alternatively, this may be written in the abbreviated form

$$^{9}Be(\alpha,n)^{12}C\tag{2.2}$$

This representation states that Be is the target nucleus, interacting with an incident alpha particle (α); a neutron (*n*) is ejected and a ${}^{12}C$ nucleus, referred as the recoil nucleus, remains. The major alpha particle emitters used in (α ,n) sources, together with beryllium, are radium-226, polonium-210, and plutonium-239. In these cases,

output neutrons have high energy range from 1 to 10 MeV or more. Such neutrons are known as polyenergetic.

On the other hand, monoenenergetic neutrons can be obtained by the action of gamma rays about 2 MeV on certain type nuclei such as deuterium, heavy hydrogen and beryllium. The reactions are given as

$${}^{9}_{4}Be + {}^{0}_{0}\gamma \longrightarrow {}^{8}_{4}Be + {}^{1}_{0}n$$

$$(2.3)$$

and

$${}^{2}_{1}H + {}^{0}_{0}g \longrightarrow {}^{1}_{1}H + {}^{1}_{0}n$$

$$(2.4)$$

These are described as (γ, n) reactions and called as photoneutron sources. This reaction occurs only if the energy of the gamma rays is at least equal to binding energy of the neutron in the target nucleus. Due to the fact that the binding energy is exceptionally low in deuterium (2.2 MeV) and beryllium (1.6 MeV) that these substances are generally used in (γ, n) neutron sources. Obtaining neutrons from other elements requires gamma rays of at least 6 to 8 MeV energy [5].

2.1.2 Neutron Absorption Reactions

Reactions of neutrons with nuclei separate into two groups, scattering and absorption. In absorption process the neutron is witholded by the nucleus and a new particle is formed. The most important absorption reaction in nuclear reactors are radiative capture and fission which will be mentioned in detail. There are also a few neutron absorption reactions of different types. In considering absorption reactions it

is convenient to distinguish between reactions of slow and of fast neutrons. There are three main kind of slow neutron reactions;

- a. Emission of gamma radiation (radiative capture) (n, γ)
- b. The ejection of a charged particle (such as (n, α) and/or (n,p) reactions)
- c. Fission (n,f)

Radiative capture occurs with a wide variety of elements. The (n, α) and (n,p) reactions, these are called charged particle emission, with slow neutrons are limited to a few isotopes of low mass number, however fission by slow neutrons is restricted to certain nuclei of high mass number.

2.1.2.A. Radiative Capture Reactions

In these reactions, excited compound nucleus emits its excess energy as gamma rays. The process may be shown like this form

$${}_{Z}X^{A} + {}_{0}n^{1} \longrightarrow [{}_{Z}X^{A+1}]^{*} \longrightarrow {}_{Z}X^{A+1} + \gamma$$

$$(2.5)$$

Having an atomic number Z and a mass A, $_ZX^A$ is the target nucleus. The product $_ZX^{A+1}$ is the isotope of $_ZX^A$ and it may be radioactive or not [5]. If it is radioactive, it will most likely be a beta emitter because the capture of a neutron will have produced a nucleus in which the neutron-to-proton ratio is too large for stability for the given atomic number. Actually all the elements show the radiative capture reaction much or less extent. However some nuclei exhibit little inclination to capture neutrons. Two example for radiative capture is uranium-238 and thorium-232, and also uranium-235 and plutonium-239 represent radiative capture, in competition with fission, especially for neutrons of intermediate and low energies. The neutron capture reaction does not require any specific neutron energy and the reaction can occur with the neutron of any energy. In this reaction the Q-value becomes positive, that is, exothermic since the binding energy of the product nucleus is larger than the summation of the binding energy of the neutron and the original nucleus.

2.1.2.B. Charged Particle Emission

A charged particle reaction, which is also called as "transmutation" reaction, usually pioneers to emission of an α particle or a proton from the nucleus. Due to the fact that a positively charged particle can be expelled from a nucleus only if it has sufficient energy to overcome an electrostatic potential, the slow-neutron reactions rarely produce the charged particles. Only for a few element of low atomic number, for which the nuclear electrostatic repulsion is small,

$${}^{10}_{5}B + {}^{1}_{0}n \longrightarrow {}^{11}_{5}B^* \longrightarrow {}^{7}_{3}Li + {}^{4}_{2}He$$

$$(2.6)$$

that charged-particle emission is possible after capture of a slow neutron. The (n, α) reaction with boron-10 can be shown as ${}^{4}_{2}He$ representing the α particle. In this reaction, the charged particles are ejected in opposite directions with relatively high energy. This is the basis of a method for detecting and counting slow neutrons. Since boron undergoes the (n, α) reaction very rapidly with slow neutrons, this element is used for controlling the reactor core like cadmium. Another reaction producing the charged particles is the (n, α) reaction of Li:

$${}_{3}^{6}Li + n \longrightarrow ({}_{3}^{7}Li)^{*} \longrightarrow {}_{1}^{3}H + {}_{2}^{4}He$$

$$(2.7)$$

This reaction is similar with the previous one. Here ${}_{1}^{3}He$ is the residual and a betaactive, hydrogen isotope of mass number 3 is called *tritium*.

2.1.2.C. Fission Reactions

Neutrons colliding with certain nuclei may cause the nucleus split apart to undergo *fission*. Fission occurs only with certain nuclei of high atomic (and mass) number, and hence the repulsive force within the nucleus is an important contributory factor. When fission occurs, the excited compound nucleus formed after absorption of a neutron breaks up into two lighter nuclei, called *fission fragments*. If the neutron is

one of low kinetic energy, i.e. a slow neutron, the two fragment nuclei generally have unequal masses. That is to say, symmetrical fission by slow neutrons is rare; in the majority of slow- neutron fissions the mass ratio of the fragments is appoximately 2 to 3.

Only three nuclides, having sufficent stability to permit storage for a long time, namely uranium-233, uranium-235, and plutonium-239, are fissionable by neutrons of all energies, from thermal values to millions of electron volts. Of these nuclides, uranium-235 is the only one which occurs in nature; the other two are produced artifically from thorium-232 and uranium-238, respectively.

In addition to the nuclides which are fissionable by neutrons of all energies, there are some other nuclides that require fast neutrons to cause fission such as thorium-232 and uranium-238. For neutrons below about 1 MeV energy, but above this theresold value, fission also occurs to some extent. Since fission of thorium-232 and uranium-238 is possible with sufficiently fast neutrons, they are known as *fissionable nuclides*. In distinction, uranium-233, uranium-235, and plutonium-239, which will undergo fission with neutrons of any energy, are referred to as *fissile nuclides*. Moreover, since thorium-232 and uranium-238 can be converted into the fissile species, uranium-233 and plutonium-239, respectively, they are also called *fertile nuclides*.

Some fertile nuclides can be converted into useful nuclear fuel for fission reactors in which most of neutrons are moving slowly. The most important two fissile breeding reactions are [6]

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

$$(2.8)$$

and

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

$$(2.9)$$

The importance of fission, from the standpoint of the utilization of nuclear energy, lies in two facts: First, the process is associated with the release of a large amount of energy per unit mass of nuclear fuel and, second, the fisson reaction, which is initiated by neutrons, is accompanied by the liberation of neutrons. It is the combination of these two circumtances that makes possible the design of a nuclear reactor in which a self-sustaining fission chain reaction occurs with the continuous release of energy. Once the fission reaction has been started in a few nuclei by means of an external source of neutrons, it can be maintained in other nuclei by the neutrons produced in the reaction. It should be noted that it is only with the fissile nuclides mentioned above that a self sustaining chain is possible. Thorium-232 and uranium-238 cannot support a fission chain because the fission probability is small even for neutrons with energies in excess of the threeshold of 1 MeV, and inelastic scattering soon reduces the engies of many neutrons below the theresold value [5].

Some typical neutron-induced fission reactions for different neutron energies are

$${}^{235}U + n \longrightarrow {}^{236}U * \longrightarrow {}^{93}Rb + {}^{141}Cs + 2n$$

$${}^{235}U + n \longrightarrow {}^{236}U * \longrightarrow {}^{137}_{53}I + {}^{96}_{39}Y + 3n$$

$${}^{235}U + n \longrightarrow {}^{236}U * \longrightarrow {}^{142}_{55}Cs + {}^{90}_{37}Rb + 4n$$

$$(2.10)$$

These reactions are possible for incident neutrons of thermal energies. [7]

2.1.3 Neutron Scattering Reactions

Neutrons having energies above the thermal range, a scattering collision results in degradation of the neutron energy. Energy degradation caused by scattering is referred to as neutron slowing down. In a medium where the average energy lose per collision and the ratio of scattering to absorption cross section is large, the neutron

spectrum becomes close to thermal equilibrium. That is referred to thermal or soft spectrum. Contrary in a system for which small degradation to absorption, neutrons are absorbed before significant slowing down takes place. Then the neutron spectrum becomes closer to the fission spectrum and is called to be hard or fast. To understand the neutron energy distribution more quantitively, we must consider first elastic and inelastic scatterings. In elastic scattering the sums of the kinetic energies of the neutrons and the target nucleus is same before and after collision. That is energy is conserved. However in inelastic collision, it is not conserved because the some of kinetic energies of nucleus and target nucleus before scattering is less or greater than after scattering. Both elastic and inelastic scattering are of considerable importance in nuclear reactors.

2.1.3.A. Elastic Scattering

In elastic scattering, the target nucleus remains in its lowest energy (ground) state, this interaction treats as a billiard ball type collision as seen in Figure 2.1. Thus, this behavior can be analyzed in terms of mechanic laws with conservation principles of both momentum and energy



Figure 2.1 Schematics of the potential elastic neutron scattering [4]

After sufficient number of elastic collisions, the velocity of neutron reduces that has approximately the same average kinetic energy as the atoms of the scattering medium. This energy depends on the temperature of the medium that is called thermal energy. Thermal neutrons are the neutrons in thermal equilibrium with the atom in the medium. A certain thermal neutron undergoing scattering collision with the nuclei of the present medium may gain or lose energy in any one collision. But, if a large number of thermal neutrons diffusing in a non-absorbing medium are considered, becomes no net energy change for all the neutrons.

There are two possible ways for a neutron to scatter elastically. The first one is resonance or compound elastic scattering: the neutron is absorbed by the target nucleus to form a compound nucleus followed by re-emission of a neutron. The other is potential elastic scattering. the short range nuclear force scatter the neutron away from the nucleus surface. The more unusual of the two interactions is the resonance elastic scattering that is highly dependent on initial neutron kinetic energy. Near the resonance energies there is a quantum mechanical interface between the potential and resonance scattering. As the neutrons approach the nucleus, they are scattered by the short range nuclear forces and is expressed by relation as σ_{el} (potential scattering)= $4\pi R^2$ where R is the radius of the nucleus [4].

2.1.3.B. Inelastic Scattering

When a fast neutron undergoes inelastic scattering, it is first captured by the target nucleus to form an excited state of the compound nucleus, then a neutron having lower kinetic energy is emitted when it leaves the target nucleus in an excited state. An excess energy becomes this energy is subsequently emitted as one or more photons of gamma radiation which is called inelastic scattering gamma rays.

If E_1 is the total kinetic energy of the neutron and target nucleus before collision and E_2 is the kinetic energy after the collision also E_{γ} is the emitted energy from gamma radiation, so,

$$E_1 = E_2 + E_{\gamma}$$

It is obvious that in inelastic scattering kinetic energy is not conserved. Nonetheless, momentum is conserved. For elements of moderate and high mass number, the energy of the lowest excited state above the ground state, is usually from 0.1 to 1MeV. When the nucleus having with decreasing mass number, becomes a general tendency for the excitation energy to increase, hence the neutrons must have higher energies if they are to undergo inelastic scattering. Due to the fact that the separation of the excited levels of a nucleus is smaller at high excitation energy. For inelastic scattering by elements of low mass number, the total gamma-ray energy must be high.

2.2. CROSS-SECTIONS and NEUTRON FLUX

Each of the reactions may occur under certain conditions and there is a need for the parameters that are used to calculate the probability if a reaction occurs or not. First, it is necessary to define the interaction area for the interacting particles.

Roughly speaking, the cross section is a measure of the relative probability for the reaction to occur. The probability that a nuclear reaction will take place is measured in units of "**barns**", where 1 barn equals 10^{-24} cm². This is a unit of area. You can visualize a target material as an array of little disks. Larger disks would be easy to hit (large cross section, large reaction probability), and smaller disks would be hard to hit.

As we mentioned above, neutron interactions with matter can be either scattering or absorption reactions. As it is well known that the scattering can result in a change in the energy and direction of motion of a neutron but cannot directly cause the disappearance of a free neutron; and the absorption leads to the disappearance of free neutrons as a result of a nuclear reaction with fission or the formation of a new nucleus and another particle or particles such as protons, alpha particles and gamma photons. The probability of occurrence of these reactions is primarily dependent on the energy of the neutrons and on the properties of the nucleus with which it is interacting.

The probability of a particular reaction occurring between a neutron and a nucleus is called the *microscopic cross section* (σ) of the nucleus for the particular reaction. This cross section will vary with the energy of the neutron. The microscopic cross section may also be regarded as the effective area the nucleus presents to the neutron for the particular reaction. The larger the effective area, the greater the probability for reaction.

Let's consider a thought experiment to determine the reaction rate R [reactions/sec] that would occur in a small volume of a thin target material of area A $[cm^2]$ and thickness x [cm] when a beam of neutrons moving in the x direction with a density n [neutrons/cm³] and velocity v [cm/sec] as shown in Fig. 2.2. If the density of the material is ρ [g/cm³], and its atomic weight is M [amu] we can use a modified form of Avogadro's law to determine the nuclei density in the target:



Figure 2.2 Geometry for neutron reaction rate in thin target of volume V.

So that the reaction rate R should be construed to be proportional to the area of the target A, its thickness x, the number density of the particles in the neutron beam, n, the velocity of the neutrons, v, and the number density of the nuclei in the target N. This can be expressed mathematically as:

$$R \propto A \times I N$$
 (Reactions/sec) (2.11)

where $\vec{I} = n \vec{v}$. The proportionality symbol can be replaced by an equality sign provided we add a proportionality constant, leading to;

$$R = \sigma A x n \vec{v} N$$
 (Reactions/sec) (2.12)

Since the volume of the target is V = Ax, then one writes

$$R^* = \frac{R}{V} = \frac{R}{Ax} = \sigma \ n \ \vec{v} \ N \ (\text{Reactions/cm}^3 \text{sec})$$
(2.13)

If the equation is rearranged for σ , we find the units of the proportionality constant as:

$$\sigma = \frac{R^*}{n \,\vec{v} \,N} \,\,(\mathrm{cm}^2) \tag{2.14}$$

Thus the proportionality constant σ has units of area and physically represents the area that a nucleus in the target presents to the interacting neutrons in the impinging beam.

The cross section is not in general equal to the actual area of the nucleus. For instance the radiative capture cross section for ¹⁹⁷Au at the peak of 4.9 eV resonance is $3x10^{-20}$ cm², whereas the geometrical area of its nucleus is just $1.938x10^{-24}$ cm². The reaction cross section is much greater than the physical cross section of the nucleus,

except at very high neutron energies where the cross section becomes of the same order of magnitude as the nucleus. This can be calculated from the knowledge about the empirically determined expression for the radius of the nucleus as:

$$r = r_0 A^{1/3}$$

$$r_0 = 1.35 \times 10^{-13} cm$$
(2.15)

then the cross sectional area is

$$s = \pi r^2 = \pi r_0^2 A^{2/3} \quad (cm^2) \tag{2.16}$$

For ¹⁹⁷Au, the area of the nucleus becomes:

$$s = \pi (1.35 \times 10^{-13})^2 (197)^{2/3}$$

$$s = 1.938 \times 10^{-24} \quad (cm^2)$$

$$s = 1.938 \, barn$$
(2.17)

It is well understood that the probability of a particular reaction occurring between a neutron and a nucleus is called the *microscopic cross section* (σ) of the nucleus for the particular reaction.

2.2.1 Microscopic Reaction Cross-Sections

Each probable reaction that a neutron can undergo with a nucleus is associated with a specific cross section. The most important of them are given in Table 2.1.

$\sigma_{f} = fission cross section \sigma_{\gamma} = radiative capture cross section \sigma_{a} = \sigma_{\gamma} + \sigma_{f} = absorption cross section $	$\left\{\sigma_t = \text{total cross section}\right\}$
$\sigma_{es} = \text{elastic scattering cross section} \\ \sigma_{in} = \text{inelastic scattering cross section} \\ \sigma_{s} = \sigma_{es} + \sigma_{in} = \text{scattering cross section} $	

The sum of the cross sections that can lead to the disappearance of the neutron is designated as the *absorption cross section*:

$$\sigma_a = \sigma_\gamma + \sigma_f + \sigma_p + \sigma_T + \sigma_\alpha \tag{2.18}$$

The sum of the cross sections that can lead to the scatterance of the neutron is designated as the *scattering cross section*: (for the elastic and inelastic scattering)

$$\sigma_s = \sigma_{se} + \sigma_{si} \tag{2.19}$$

and the total cross section is written as:

$$\sigma_t = \sigma_a + \sigma_s \tag{2.20}$$

2.2.2 Macroscopic Reaction Cross-Sections

Whether a neutron will interact with a certain volume of material depends not only on the microscopic cross section of the individual nuclei but also on the number of nuclei within that volume. Most materials are composed of several elements, and because most elements are composed of several isotopes, most materials involve many cross sections, one for each isotope involved. Therefore, to include all the isotopes within a given material, it is necessary to determine the *macroscopic cross* section (Σ) for each isotope and then sum all the individual macroscopic cross sections. The *macroscopic cross section* is the probability of a given reaction occurring per unit travel of the neutron [1]. It is related to the *microscopic cross* section (σ) by the relationship

$$\Sigma = N \sigma \tag{2.21}$$

where:

 Σ = macroscopic cross section (cm⁻¹)

N = atom density of material ($atoms/cm^{-3}$)

 σ = microscopic cross-section (barn)

The difference between the microscopic and macroscopic cross sections is extremely important and is restated for clarity. The microscopic cross section (σ) represents the effective target area that a single nucleus presents to a bombarding particle. The units are given in barns or cm^2 . The macroscopic cross section (Σ) represents the effective target area that is presented by all of the nuclei contained in 1 cm^3 of the material. The units are given as 1/cm or cm^{-1} .

Equation (2-21) can be used to determine the macroscopic cross section for a composite material:

$$\Sigma = N_1 \sigma_1 + N_2 \sigma_2 + N_3 \sigma_3 + \dots + N_n \sigma_n \tag{2.22}$$

where

N is the number nuclei per cm³ of the nth element,

 σ is the microscopic cross section of the nth element.

2.2.3 Neutron Flux

Suppose a thick target of thickness X is placed in a monodirectional beam of intensity I_0 and a neutron detector is located at some distance behind the target. Every neutron that has a collision in the target is lost from the beam, and only those neutrons that do not interact enter the detector behind the target. Let I(x) be the intensity of the neutrons that have <u>not</u> collided after penetrating the distance x into the target. Then in traversing the additional distance dx, the intensity in the thin sheet of target having an area of 1 cm^2 and the thickness dx. By using the equation (2.12), this decrease in intensity is given by

$$-dI(x) = N \sigma_t I(x) dx = \Sigma_t I(x) dx$$
(2.23)

This equation can be integrated and we get

$$I(x) = I_0 e^{-\Sigma_t x}$$
(2.24)

Thus, the intensity of the neutrons uncollided with the target nuclei is given by

$$I(X) = I_0 e^{-\Sigma_t x}$$
(2.25)

Since the Σ_t is the probability of interaction per path length, p(x)dx is

$$p(x) dx = e^{-\Sigma_t x} \times \Sigma_t dx$$
(2.26)

and the average distance that a neutron moves between collisions is called the mean free path, and it is equal to the average value of x, the distance traversed by a neutron without any collision. So we get,

$$\lambda = \int_{0}^{\infty} xp(x) dx$$

$$\lambda = \sum_{t} \int_{0}^{\infty} x e^{-\Sigma_{t} x} dx$$

$$\lambda = 1 / \Sigma_{t}$$
(2.27)

Since a beam of neutrons of intensity I strikes a thin target, the number of collisions per unit volume per time is given by

$$F = I \Sigma_t \tag{2.28}$$

where Σ_t is the macroscopic total cross-section. Let's consider an experiment in which a target is exposed simultaneously to several neutrons beams. Assume the intensities of the beams are different but the neutrons have the same energy. The beam's directions are different. Then, the total interaction rate is given by

$$F = \Sigma_t (I_A + I_B + I_C + \cdots)$$
(2.29)

Since the neutrons are monoenergetic, then Eq. (2.29) becomes

$$F = \Sigma_t (n_A + n_B + n_C + \cdots) v \tag{2.30}$$

where n_A, n_B, n_C are the densities of neutrons with speed of v. Since $n_A + n_B + n_C + \cdots$ is equal to the total n, then

$$F = \Sigma_t \ n \ v \tag{2.31}$$

The situation at any point in a reactor is a generalization of this experiment, but with the neutrons moving in *all* directions. Eq. (2.31) is valid for any reactor.

The quantity nv is called the *neutron flux*, in this case for monoenergetic neutrons, and is given by the symbol ϕ . Then the collision density is given by

$$F = \sum_{t} \phi \tag{2.32}$$

We now extend this result to include neutrons that have a distribution of energies. Thus consider n(E) be defined as the neutron density per unit energy; that is, n(E)dE is the number of neutrons per cm³ with energies between E and E + dE. From Eq. (2.32) the interaction rate for these essentially monoenergetic neutrons is

$$dF = \sum(E) \times n(E) dE \times v(E)$$
(2.33)

where energy dependence of all parameters is noted explicity. The total interaction rate is then given by the integral

$$F = \int_{0}^{\infty} \sum_{t} (E) n(E) \upsilon(E) dE = \int_{0}^{\infty} \sum_{t} (E) \phi(E) dE$$
(2.34)

where

$$\phi(E) = n(E)\upsilon(E) \tag{2.35}$$

This equaiton is called the energy-dependent flux or the flux per unit energy. The limit of this equation is indicated that the integration is examined over all neutron energies and Eq. (2.34) shows the total interaction rate. Specific interaction rates can be found similar way. The number of scattering collision rate is

$$F_s = \int_0^\infty \sum_s (E)\phi(E)dE$$
(2.36)

and the absorption interaction rate per cm^3/s is

$$F_a = \int_0^\infty \sum_a (E)\phi(E)dE$$
(2.37)

2.2.4 Fick's Law:

The neutrons in a reactor move about in complicated paths as the result of repeated nuclear collisions. To a first approximation, the overall effect of these collisions is that the neutrons undergo a kind of diffusion in the reactor medium, much like the diffusion of one gas in another. The approximate value of the neutron distribution can be found by solving the diffusion equation – essentially the same equation used

to describe diffusion phenomena in other branches of engineering such as molecular transport. This procedure is called the diffusion approximation. Diffusion theory is based on Fick's law [8].

The diffusion theory of neutron transport plays a crucial role in reactor theory since it is simple enough to allow scientific insight, and it is sufficiently realistic to study many important design problems. The neutrons are here characterized by a single energy or speed (that means they are monoenergetic), and the model allows preliminary design estimates. The mathematical methods used to analyze such a model are the same as those applied in more sophisticated methods such as multigroup diffusion theory, and transport theory. The derivation of the diffusion equation will depend on *Fick's law*, even though a direct derivation from the transport equation is also possible. The Helmholtz equation is derived, and the limitations on diffusion equation as well as the boundary conditions used in its application to realistic problems are discussed.

The neutron flux (ϕ) and current (\vec{J}) are related in a simple way under certain conditions. This relationship between ϕ and \vec{J} is identical in form to a law used in the study of diffusion phenomena in liquids and gases: *Fick's Law*. In Physical Chemistry, Fick's law states that: "If the concentration of a solute in one region is greater than in another of a solution, the solute diffuses from the region of higher concentration to the region of lower concentration." The use of this law in reactor theory leads to the diffusion approximation. Let us make the following assumptions:

- 1. We consider an infinite medium.
- The cross sections are constants, independent of position, implying a uniform medium.
- 3. Scattering is isotropic in the Laboratory (LAB) system.
- 4. The neutron flux is a slowly varying function of the position.
- 5. We use a one speed system where the neutron density is not a function of energy.
- 6. A steady state system where the neutron density is not a function of time.
- 7. No fission source in the system.

Later, some of these assumptions will be relaxed. For instance, the diffusing medium will be taken as finite in size rather than infinite. Now, we shall attempt to calculate the current density at the center of the coordinate system in Figure 2.3.



Figure 2.3 Geometry for the derivation of the neutron current and Fick's Law [8].

In a cartesian coordinate system given in Figure 2.3, we consider an infinite medium in which neutrons are diffusing and being scattered, with an element of volume dVwhose position is defined by the vector \vec{r} , and an element area of dA lying in the x-y plane at the origin of the coordinate system. Let the neutron flux at \vec{r} be $\phi(\vec{r})$. Then, the neutron current density vector \vec{J} is given by:

$$\vec{J} = J_x \hat{i} + J_y \hat{j} + J_z \hat{k}$$
(2.38)

So that we must determine the components of \vec{J} . These net current components can be written in terms of the partial axial currents as:

$$J_{x} = J_{x}^{+} - J_{x}^{-}$$

$$J_{y} = J_{y}^{+} - J_{y}^{-}$$

$$J_{z} = J_{z}^{+} - J_{z}^{-}$$
(2.39)

Let us concentrate on the estimation of one single component: J_z crossing the element of area dS_z at the origin of the coordinate system in the negative *z* direction, as shown in Fig. 2.3. Every neutron passing through dS_z in the *x*-*y* plane comes from a scattering collision. A neutron scattering above the *x*-*y* plane will thus flow downward through dS_z .

Consider the volume element:

$$dV = r^2 \sin(\theta) dr \, d\theta \, d\phi \tag{2.40}$$

The number of scattering collisions occurring per unit time in the volume element dV is:

$$\sum_{s} \phi(\vec{r}) dV = \sum_{s} \phi(\vec{r}) r^{2} \sin(\theta) dr d\theta d\phi$$
(2.41)

where \sum_{s} is the macroscopic scattering cross section, and $\phi(\vec{r})$ is the particle flux in three dimensions. Since scattering is isotropic in the LAB system, the fraction arriving to dSz is that subtended by the solid angle d Ω , given by:

$$\frac{d\Omega}{\Omega} = \frac{\frac{dS}{r^2}}{4\pi} = \frac{dS_z \cos(\theta)}{4\pi r^2}$$
(2.42)

Thus the number of neutrons scattered per unit time in dV reaching dSz after being attenuated in the medium by the exponential factor $e^{\sum_{t} r}$ is:

$$dN = e^{\sum_{t} r} \sum_{s} \phi(\vec{r}) r^{2} \sin(\theta) dr d\theta d\phi \frac{dS_{z} \cos(\theta)}{4\pi r^{2}}$$
(2.43)
The partial current J_z^- can now be written as:

$$J_{z}^{-} = \int \frac{dN}{dS_{z}} = \frac{\sum_{s}}{4\pi} \int_{0}^{\infty} \int_{0}^{\pi/2} \int_{0}^{2\pi} e^{\sum_{t} r} \phi(\vec{r}) \sin(\theta) \cos(\theta) dr d\theta d\phi \qquad (2.44)$$

Since $\phi(\vec{r})$ is an unknown function, we expand it in a Taylor's series assuming it varies slowly with position:

$$\phi(\vec{r}) \cong \phi_0 + x \frac{\partial \phi}{\partial x}\Big|_{x=0} + y \frac{\partial \phi}{\partial y}\Big|_{y=0} + z \frac{\partial \phi}{\partial z}\Big|_{z=0} + \dots$$
(2.45)

Writing x, y, z in spherical coordinates, we get

$$\phi(\vec{r}) \cong \phi_0 + r\sin(\theta)\cos(\phi)\frac{\partial\phi}{\partial x}\Big|_{x=0} + r\sin(\theta)\sin(\phi)\frac{\partial\phi}{\partial y}\Big|_{y=0} + r\cos(\theta)\frac{\partial\phi}{\partial z}\Big|_{z=0}$$
(2.46)

Substituting Eq. (2.46) into Eq. (2.44), we write,

$$J_{z}^{-} = \int \frac{dN}{dS_{z}} = \frac{\sum_{s}}{4\pi} \int_{0}^{\infty} \int_{0}^{\pi/2} \int_{0}^{2\pi} e^{\sum_{r} r} \begin{bmatrix} \phi_{0} + r\sin(\theta)\cos(\varphi)\frac{\partial\phi}{\partial x}\Big|_{x=0} + r\cos(\theta)\frac{\partial\phi}{\partial z}\Big|_{x=0} \\ r\sin(\theta)\sin(\varphi)\frac{\partial\phi}{\partial y}\Big|_{y=0} + r\cos(\theta)\frac{\partial\phi}{\partial z}\Big|_{z=0} \end{bmatrix} \sin(\theta)\cos(\theta)drd\theta d\varphi^{(2.47)}$$

The terms containing $\cos(\varphi)$ and $\sin(\varphi)$ are integrated to zero over the interval $\varphi \in [0, 2\pi]$. Thus we get

$$J_{z}^{-} = \int \frac{dN}{dS_{z}} = \frac{\sum_{s}}{4\pi} \int_{0}^{\infty} \int_{0}^{\pi/2} \int_{0}^{2\pi} e^{\sum_{t} r} \left[\phi_{0} + r \cos(\theta) \frac{\partial \phi}{\partial z} \Big|_{z=0} \right] \sin(\theta) \cos(\theta) dr d\theta d\phi \quad (2.48)$$

The first term can be evaluated as:

$$I_{1} = \frac{\sum_{s}}{4\pi} \int_{0}^{\infty} \int_{0}^{\pi/2} \int_{0}^{2\pi} \phi_{0} e^{\sum_{t} r} \sin(\theta) \cos(\theta) dr d\theta d\varphi$$

$$I_{1} = \frac{\sum_{s}}{4\pi} \phi_{0} 2\pi \frac{1}{\sum_{t}} \frac{1}{2}$$

$$I_{1} = \frac{1}{4} \frac{\sum_{s}}{\sum_{t}} \phi_{0}$$
(2.49)

Then second term is:

$$I_{2} = \frac{\sum_{s} \left. \frac{\partial \phi}{\partial z} \right|_{z=0} \int_{0}^{\infty} \int_{0}^{\pi/2} \int_{0}^{2\pi} e^{\sum_{t} r} r \sin(\theta) \cos^{2}(\theta) dr d\theta d\phi$$

$$I_{2} = \frac{\sum_{s} \left. \frac{\partial \phi}{\partial z} \right|_{z=0} 2\pi \frac{1}{\sum_{t}^{2}} \frac{1}{3}$$

$$I_{2} = \frac{1}{6} \frac{\sum_{s} \left. \frac{\partial \phi}{\partial z} \right|_{z=0} \left. \left. \frac{\partial \phi}{\partial z} \right|_{z=0}$$
(2.50)

As a result, the Eq. (2.48) is written as

$$J_{z}^{-} = \frac{1}{4} \frac{\sum_{s}}{\sum_{t}} \phi_{0} + \frac{1}{6} \frac{\sum_{s}}{\sum_{t}^{2}} \frac{\partial \phi}{\partial z} \bigg|_{z=0}$$
(2.51)

If the same procedure is done for J_z^+ then we get

$$J_{z}^{+} = \frac{1}{4} \frac{\sum_{s}}{\sum_{t}} \phi_{0} - \frac{1}{6} \frac{\sum_{s}}{\sum_{t}^{2}} \frac{\partial \phi}{\partial z} \bigg|_{z=0}$$
(2.52)

Similarly, the other current values can be obtained, and substituting the results into the Eq. (2.39), we can write

$$J_{x} = -\frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}} \frac{\partial \phi}{\partial x} \Big|_{x=0}$$

$$J_{y} = -\frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}} \frac{\partial \phi}{\partial y} \Big|_{y=0}$$

$$J_{z} = -\frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}} \frac{\partial \phi}{\partial z} \Big|_{z=0}$$
(2.53)

Substituting into Eq. (2.38), we get the expression for the current density after dropping the evaluation at the origin notation, since the origin of the coordinates is arbitrary:

$$\vec{J} = -\frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}} \left(\frac{\partial \phi}{\partial x} \Big|_{x=0} \hat{i} + \frac{\partial \phi}{\partial y} \Big|_{y=0} \hat{j} + \frac{\partial \phi}{\partial z} \Big|_{z=0} \hat{k} \right)$$

$$\vec{J} = -\frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}} \left(\frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k} \right) \phi$$

$$\vec{J} = -\frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}} \vec{\nabla} \phi = -\frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}} \operatorname{grad} \phi$$
(2.54)

In the last equation, we define the "diffusion coefficient":

$$D = \frac{1}{3} \frac{\sum_{s}}{\sum_{t}^{2}}$$
(2.55)

Thus Fick's law for neutron diffusion is given by:

$$\vec{J} = -D\vec{\nabla}\phi \tag{2.56}$$

It states that the current density vector is proportional to the negative gradient of the flux, and establishes a relationship between them under the enunciated assumptions.

Notice that the gradient operator turns the neutron flux, which is a scalar quantity into the neutron current, which is a vector quantity, see Fig. 2.4 and Fig. 2.5.



Figure 2.4 Neutron flux and current.

It must be emphasized that Fick's law is not an exact relation. It expresses the fact that if the gradient of the flux is negative, then the current density is positive. This means that the particles will diffuse from the region of higher flux to the region of lower flux through collisions in the medium.

The Fick's Law is just an approximation, then it is in particular not valid under the following conditions:

- 1. In a medium that strongly absorbs neutrons,
- 2. Within about three mean free paths of either a neutron source or the surface of a medium,
- 3. When the scattering of neutrons is strongly anisotropic.

The parameter of *Diffusion Coefficient* given in Eq. (2.55) can be calculated approximately by a more easy formula:

$$D = \frac{1}{3\sum_{s}(1-\bar{\mu})(1-\frac{4}{5}\frac{\sum_{a}}{\sum_{t}}+...)}$$
(2.57)



Figure 2.5 Neutron flux and current in the wall of reactor.

If $\sum_{a} \ll \sum_{t}$ then it can be written as

$$D = \frac{1}{3\sum_{s}(1-\bar{\mu})} = \frac{1}{3\sum_{tr}} = \frac{\lambda_{tr}}{3}$$
(2.58)

Since $\sum_{s} (1 - \overline{\mu}) = \sum_{tr} = 1/\lambda_{tr}$ where λ_{tr} is the transport mean free path and \sum_{tr} is called macroscopic transport cross-section and \sum_{s} is the macroscopic crosssection of the medium, and m is the average value of the cosine of the angle at which neutrons are scattered in the medium in the laboratory system. The value of $\overline{\mu}$ is computed in reactor calculations by a simple equation as [2, 4, 9] $\overline{\mu} = \frac{1}{3A}$ where A is the mass number.

CHAPTER 3

SOLUTION OF DIFFUSION EQUATION FOR

NON-MULTIPLYING SYSTEMS

3.1 EQUATION OF CONTINUITY

Assume an arbitrary volume V within a medium containing neutrons. As time, neutron number in volume may change if there is a net flow of neutrons out of or into that volume: If some of the neutrons are absorbed within the volume and leakage from the volume, or if some sources emitting neutrons are present within that volume. Then, the equation of continuity can be a mathematical statement that the time rate of change in the number of neutrons in that volume must be accounted for in terms of these processes since neutrons do not disappear unaccountably: Therefore, one can write

$$\begin{bmatrix} rate of change in \\ number of neutrons in V \end{bmatrix} = \begin{bmatrix} rate of production \\ of neutrons in V \end{bmatrix} + \begin{bmatrix} rate of fission of \\ neutrons in V \end{bmatrix} \\ - \begin{bmatrix} rate of leakage of \\ neutrons from V \end{bmatrix} - \begin{bmatrix} rate of absorption \\ of neutrons in V \end{bmatrix}$$
(3.1)

Each of these terms is considered in the followings:

Let n be the density of neutrons at any point and time in V. The total number of neutrons in V is then

$$\int_{V} n \, dV, \tag{3.2}$$

where the subcript on the integral indicates that the integration is to be performed throughout V. The rate of chance in number of neutrons is

$$\frac{d}{dt} \int_{V} n dV, \qquad (3.3)$$

which can also be written as

$$\int_{V} \frac{\partial n}{\partial t} dV. \tag{3.4}$$

let *s* be the rate at which neutrons are emitted from sources per cm³ in *V*. The rate at which neutrons are produced throughout *V* is given by

$$Production \, rate = \int_{v} s dV. \tag{3.5}$$

The rate of neutrons produced by fission, contributes to source is equal to $\nu \sum_f \phi$, per cm³/sec. \sum_f is the macroscopic fission cross section, over all the volume the total produced of neutrons by fission becomes [2]

$$Fission \, rate = \int_{V} \upsilon \sum_{f} \phi dV \tag{3.6}$$

Consider that the flow of neutrons into and out of V. If \vec{J} is neutron current density vector through the surface of a volume V and **n** is a unit normal pointing outward from the surface, then the net number of neutrons passing outward through the surface per cm²/sec is define by

It follows that the total rate of leakage of neutrons (which may be positive or

 $\vec{J} \, \Box \vec{n}$

negative) through the surface A of the volume is

$$Leakage \ rate = \int_{v} \vec{J} \, \Box \vec{n} \, dA. \tag{3.8}$$

(3.7)

This surface integral can be transformed into a volume integral by using the divergence theorem (see Appendix A for details):

$$\int_{A} \vec{J} \,\Box \vec{n} \, dA = \int_{V} div \, \vec{J} \, dV, \tag{3.9}$$

and so

$$Leakage \, rate = \int_{v} div \, \vec{J} \, dV. \tag{3.10}$$

The rate at which neutrons are lost by absorption per cm³/sec is equal to $\sum_{a} \phi$, where \sum_{a} is the macroscopic absorption cross-section (which may be a function of position) and ϕ is the neutron flux. Throughout the volume V, the total loss of neutrons per second due to absorption is then

Absorption rate =
$$\int_{V} \sum_{a} \phi \, dV \tag{3.11}$$

The equation of continuity can now be obtained by introducing the prior results into equation Eq.(3.1). This gives us

$$\int_{v} \frac{\partial n}{\partial t} dV = \int_{v} s dV + \int_{v} v \sum_{f} \phi dV - \int_{v} \sum_{a} \phi dV - \int_{v} div J dV.$$
(3.12)

All of the previous integrals are to be caried out over the same volume, and so their integrands must be equal. The equation must hold for any arbitrary volume. Therefore, the integrands on the right when summed must be equal to the integrand on the left. Thus,

$$\frac{\partial n}{\partial t} = s + \upsilon \sum_{f} \phi - \sum_{a} \phi - divJ.$$
(3.13)

Equation (3.13) is the general form of the equation of continuity. If the neutron density is not a function of time, this equation reduces to

$$divJ + \sum_{a} \phi - s - \upsilon \sum_{f} \phi = 0 \tag{3.14}$$

which is kown as the steady-state equation of continuity [1-4].

3.2 THE DIFFUSION EQUATION

We need to develop a one-speed diffusion theory mathematical description of nuclear reactors. Such a relatively simple description has the great advantage of illustrating many of the important features of nuclear reactors without the complexity that is introduced by the treatment of important effects associated with the neutron energy spectrum and with highly directional neutron transport, which are the subjects of subsequent chapters. Moreover, diffusion theory is sufficiently accurate to provide a

quantitative understanding of many physics features of nuclear reactors and is, in fact, the workhorse computational method of nuclear reactor physics.

It is developed a neutron balance equation for unit volume of a medium in which neutrons are being produced, absorbed and are diffusing at constant energy. The rate of change of the neutron density is equal to the rate at which neutrons are produced per unit volume in the medium minus the sum of the rates of neutron leakage and absorption per unit volume in the medium. In the previous section, an equation called the continuity equation has been obtained for the process. Unfortunately, the continuity equation has two unknowns –the neutron density, n, and the neutron current density vector, \vec{J} . In the Fick's Law, a relationship has been obtained between the current and the flux: $\vec{J} = -D\vec{\nabla}\phi$. By substituting this relation into the continuity equation, one obtains the neutron diffusion equation:

$$\frac{\partial n}{\partial t} = s + \upsilon \sum_{f} \phi - \sum_{a} \phi - div(-D\vec{\nabla}\phi)$$
(3.15)

where the constant D is not a function of position and $\vec{\nabla}$ is gradient operator (see Appendix A for details). If the equation is rearranged, then we get the neutron diffusion equation in explicit form:

$$\frac{\partial n}{\partial t} = s + \upsilon \sum_{f} \phi - \sum_{a} \phi + D\nabla^{2} \phi$$
(3.16)

where ∇^2 is called *Laplacian* (see Appendix A for details). The Laplacian is written in different forms for various coordinate systems. Now, the flux can be assumed to be $\phi = n v$, where v is the constant speed of neutrons. If this is replaced into the last equation, we find

$$\frac{1}{\nu}\frac{\partial\phi}{\partial t} = s + \upsilon \sum_{f} \phi - \sum_{a} \phi + D\nabla^{2}\phi$$
(3.17)

Since we deal with the time-independent conditions, then we can write

$$D\nabla^2 \phi + s + \upsilon \sum_f \phi - \sum_a \phi = 0$$
(3.18)

This is the steady-state diffusion equation. It is more useful to write the equation in a convenient form as

$$\nabla^2 \phi - \frac{1}{L^2} \phi = -\frac{s}{D} - \frac{1}{L^2} k_{\infty} \phi$$
(3.19)

where k_{∞} is the infinite medium multiplication factor equal to $k_{\infty} = v \sum_{f} / \sum_{a}$ the parameter L^{2} is given by $L^{2} = \frac{D}{\sum_{a}}$ and called as the *diffusion area*, quantity L itself is called as the *diffusion length*. The diffusion length is a very important parameter in nuclear engineering and its significance will be given in the following examples.

The solution of the diffusion equation must satisfy certain boundary and other conditions.

It is summarized as followings:

1. Since the equation is a partial differential equation, it is obviously necessary to specify the neutron flux and its properties. Since a negative or imaginary flux function is meaningless, then the neutron flux must be finite and non-negative at all points where the diffusion equation applies. The condition of finite flux does not necessarily apply at points where localized neutron sources exist as the diffusion equation itself is not valid at such points. 2. In a system which has a plane, line or point of symmetry, the neutron flux is symmetrical about such a plane, line or point.

3. At an interface between two different media the neutron current density normal to the interface and the neutron flux are both continuous across the interface.

$$\phi_A = \phi_B \tag{3.20}$$

$$\vec{J}_A = \vec{J}_B$$

Note that the gradient of the flux $d\phi/dx$ is not continuous across the boundary. That is:

$$\vec{J} = -D\vec{\nabla}\phi \tag{3.21}$$

If \vec{J} and ϕ are continuous, then $d\phi/dx$ will change abruptly because the value of D, the diffusion constant, is different for each medium. Hence, there will be a change in the slope of the flux at the interface.

4. At the free surface of a medium the neutron flux varies in such a way that if it is extrapolated beyond the free surface it becomes zero at a fixed distance, known as the extrapolation distance.

It is obvious that the conditions 1 and 2 are more or less self-evident. One can apply these two conditions by the equations of current density in "–" and "+" directions for any coordinate axis at the boundary layer of two different media.

In the derivation of neutron current density, it has been pointed out that the Fick's law is not valid in the immediate vicinity of some surfaces such as a surface between the medium and the atmosphere (or vacuum). It follows that the diffusion equation is

not valid. If the flux calculated from the diffusion equation assumed to vanish at a small distance d beyond the surface, then the flux determined from the diffusion equation is very nearly equal to the exact flux in the interior of the medium, see Figure 3.1. This is obviously nonphysical assumption but it is a convenient mathematical approximation that provides a high degree of accuracy for estimates of the flux inside the medium. The parameter d is called as the *extrapolation distance* (Appendix B) and given mostly as

$$d = 0.71\lambda_{tr} \tag{3.22}$$

where λ_{tr} is the transport mean free path of the medium [1] and given by $\lambda_{tr} = 3D$. Then, one gets

$$d = 2.13D$$
 (3.23)

For most media, the diffusion coefficient is about $1 \ cm$, and the extrapolation distance is about $2 \ cm$. Many reactors are a few meters in size, and the extrapolation distance can be neglected by comparison with this size.



Figure 3.1 Extrapolation distance

3.3 SOLUTION OF THE DIFFUSION EQUATION IN NON-MULTIPLYING SYSTEMS

In these systems it is necessary trying to understand diffusion treatment so that one can try to solve diffusions equations for nonmultiplying systems. That is, one can firstly consider the medium in which there is no fissionable material.

3.3.1 Infinite Planer Source

Firstly an infinite planer source is considered emitting S neutrons per cm^2/sec in infinite diffusing medium as shown in Figure 3.2.



Figure 3.2: Planer source at origin x=0

The Figure shows that there is no variation in the y or z directions, so, the flux changes do not occur. In this case flux has only be a function of x- the distance from the plane. Another examination is the symmetry about x=0 point. Then the solution may be divided into two parts for x>0 and x<0. Due to having no neutron sources present except at $x\neq 0$,

$$div J + \sum_{a} \phi + s = 0 \tag{3.24}$$

which is known as the steady state equation of continuity. On sustitution of Fick's law into the equation of continuity, neutron diffusion equation is obtained

$$D\nabla^2 \phi - \sum_a \phi + s = 0 \tag{3.25}$$

This is the steady state diffusion equation where D is the diffusion coefficient and ∇^2 is called laplacian. Formulas laplacian can be applied for various coordinate systems in here we are examining a plane so the laplacian for cartesian coordinate becomes

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$
(3.26)

It is more convenient to divide the equation by D, and the diffusion length L is $L = \sqrt{D / \sum_{a}}$ which gives

$$\nabla^2 \phi - \frac{1}{L^2} \phi = 0, \quad x \neq 0$$
 (3.27)

Because of the symmetry we may only solve the one half of the plane of the equation. The general solution of Eq. (3.27) is

$$\phi = Ae^{x/L} + Ce^{-x/L} \tag{3.28}$$

where *A* and *C* are constants (we didn't here assign *B* because *B* has a different meaning in nuclear engineering) to be determined from boundary conditions. Our equation is second order differential equation so we need two boundary conditions. Suppose that we want to solve for the problem domain that is a semi infinite medium occupying the space $0 \le x \le \infty$. If no neutrons are entering from the right, then all of the neutrons entering from the left will be absorbed as they diffuse to the right, requiring

that $\phi(\infty)=0$, we thus have two needed boundary conditions. Inserting them into Eq. (3.28)

$$\phi(\infty) = Ae^{\infty/L} + Ce^{-\infty/L} = 0$$
(3.29)

Since the flux must vanish at infinity, Eq. (3.29) can be satisfied only if A=0. Then one finds

$$\phi = Ce^{-x/L} \tag{3.30}$$

To find C the second boundry condition is applied. In the limit, x goes to zero, the net flow must approach S the source density of the plane. It follows that

$$\lim_{x \to {}^{+}0} J(x) = \frac{S}{2}$$
(3.31)

This relation is known as a source condition and is useful for other situations as well from Fick's law

$$J = -D\frac{d\phi}{dx} = \frac{DC}{L}e^{-x/L}$$
(3.32)

Inserting into Eq. (3.31) and taking the limit one gets

$$C = \frac{SL}{2D} \tag{3.33}$$

From Eq. (3.30) the flux is found to be

$$\phi = \frac{SL}{2D} e^{-|\mathbf{x}|/L} \tag{3.34}$$

Because of symmetry, the flux must be the same at "-x" and "+x" thus the solution for all points in the x-axis can be obtained by replacing x by its absolute value /x/.

3.3.2 Point Source

One can now assume that a point source S is located at the origin of an infinite medium which is extending from r=0 to $r=\infty$. So the point source is taken in spherical coordinate system that depends only on r. Then the Laplacian expressed in spherical coordinates the diffusion equation becomes for $r \neq 0$,

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\phi}{dr} - \frac{1}{L^2}\phi = 0$$
(3.35)

To solve Eq. (3.35), one identifies a new variable, ω , defined by

$$\omega = r\phi \tag{3.36}$$

Substituting in Eq. (3.35) the following equation is found for ω :

$$\omega = Ae^{-r/L} + Ce^{r/L} \tag{3.37}$$

and ϕ is found to be

$$\phi(r) = A \frac{e^{-r/L}}{r} + C \frac{e^{r/L}}{r}$$
(3.38)

where A and C are constants again and can be found by two boundry conditions applied. Firstly, if r goes to infinite, the flux must be zero. So C becomes zero. A is found from source condition, that is in the limit as $r \rightarrow 0$. Emerging from all sphere with a surface area= $4\pi r^2$, must just be equal to the source strength. Thus

$$\lim_{r \to 0} 4\pi r^2 j_r(r) = S$$

$$j_r(r) = -D \frac{d}{dr} \phi(r) = DA \left(\frac{1}{rL} + \frac{1}{r^2}\right) e^{-r/L}$$
(3.39)

and then one can determine the constant A as

$$A = \frac{S}{4\pi D} \tag{3.40}$$

Combining equations (3.38) and (3.40) the flux distribution function is found as:

$$\phi(r) = \frac{S \ e^{-r/L}}{4\pi D \ r}$$
(3.41)

Clearly all of the neutrons produced by the point source must be absorbed in the infinite medium. Taking an incremental volume as $dV=4\pi r^2 dr$, it is shown that

$$\int_{all \ space} \sum_{a} \phi(r) dV = S \tag{3.42}$$

3.3.3 Bare Slab

Assume that an infinite slab of thickness 2a which has an infinite planer source at its center emits S neutrons per cm²/sec as shown in Figure 3.3 shown below. The

diffusion equation of this system is same with Eq. (3.27) when $x \neq 0$, and also the left half plane and then right half plane has equal flux because of symmetry.



Figure 3.3 Infinite slab with planar source at x=0

Now, however, the condition on the flux as $|\mathbf{x}| \rightarrow \infty$ must be diffirent because here the flux is vanished at the extrapolated surfaces of the slab, that is, at $\tilde{x} = a + d$ for the right half plane and at $-\tilde{x} = -a - d$ for the left half of the plane where d is the extrapolated distance which is equal to d=2.13D. The solution is obtained as

$$\phi = Ae^{-x/L} + Ce^{x/L} \tag{3.43}$$

The boundary conditions are

$$\phi(a+d) = \phi(-a-d) = 0 \tag{3.44}$$

Then in view of boundary condition at a +d,

$$\phi(a+d) = Ae^{-(a+d)/L} + Ce^{(a+d)/L} = 0$$
(3.45)

so that

$$C = -Ae^{-2(a+d)/L} (3.46)$$

If we substitute this result into Eq (3.43)

$$\phi = A \left[e^{-x/L} - e^{x/L - 2(a+d)/L} \right]$$
(3.47)

The constant A is found from source condition when the limit x goes to zero, current density becomes equal to the source

$$\lim_{x \to 0} J(x) = \frac{S}{2}$$
(3.48)

then

$$A = \frac{SL}{2D} (1 + e^{-(a+d)/L})^{-1}$$
(3.49)

For positive x, therefore, $\phi(x)$ is given by

$$\phi(x) = \frac{SL}{2D} \frac{e^{-x/L} - e^{x/L-2(a+d)/L}}{1 + e^{-2(a+d)/L}}$$
(3.50)

In view of the symmetry, a solution valid for all x is obtained by substituting |x| for x; hence

$$\phi(x) = \frac{SL}{2D} \frac{e^{-|x|/L} - e^{|x|/L - 2(a+d)/L}}{1 + e^{-2(a+d)/L}}$$
(3.51)

This solution may be written in more convenient form if the numerator and denominator are multiplied by $e^{(a+d)/L}$. This gives

$$\phi(x) = \frac{SL}{2D} \frac{\sinh[(a+d-|x|)/L]}{\cosh[(a+d)/L]}$$
(3.52)

where one can use the trigonometric porperties $\frac{e^{x}-e^{-x}}{2} = \sinh(x)$ and $\frac{e^{x}+e^{-x}}{2} = \cosh(x)$.

3.3.4 Two Region Example for Sphere with Source

Now assume that system has two regions same infinite planer source but has distributed source. It shows the treatment of the boundary condition at the origin and also interface conditions. Consider a sphere of radius R with material properties D and Σ_a includes a uniform source S. The sphere is surrounded with by a second source free medium with properties D and Σ_a that extends to $r=\infty$. Our aim is now to determine the neutron flux. For this aim we write the diffusion equation as

$$-\frac{1}{r^{2}}\frac{d}{dr}r^{2}\frac{d}{dr}\phi(r) + \frac{1}{L^{2}}\phi(r) = \frac{S}{D} \qquad 0 \le r \le R$$
(3.53)

and

$$-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\phi(r) + \frac{1}{\tilde{L}^2}\phi(r) = 0 \quad R < r \le \infty$$
(3.54)

where \hat{L} is the outside medium diffusion length, within the sphere we must apply general and particular solutions for Eq. (3.53)

$$\phi(r) = \phi_g(r) + \phi_p(r) \quad 0 \le r < R \tag{3.55}$$

for a uniform source the particular solution is constant. Thus

$$\phi_p = \frac{L^2 S}{D} = \frac{S}{\sum_a} \tag{3.56}$$

The general solution is same as the solution of the point source given in Eq. (3.38) and inserting $\phi_g(r)$ and $\phi_p(r)$ into Eq. (3.55) one gets

$$\phi(r) = \frac{A}{r} \exp(r/L) + \frac{C}{r} \exp(-r/L) + \frac{S}{\sum_{a}} \quad 0 \le r < R$$
(3.57)

The solution of Eq. (3.54) has the same form as Eq. (3.38)

$$\phi(r) = \frac{A'}{r} e^{r/\bar{L}} + \frac{C'}{r} e^{-r/\bar{L}} \quad R < r \le \infty$$
(3.58)

where $\hat{L} = \sqrt{\hat{D} / \hat{\Sigma}_a}$.

Now one has two flux functions for two regions and in these equations there are four coefficients. So one must apply four boundary and interface conditions and \hat{D} symbolizes the outside medium diffusion coefficient.

1.
$$0 < \phi(0) < \infty$$
 # 2. $\phi(\infty) = 0$
3. $\phi(\mathbf{R}_{-}) = \phi(\mathbf{R}_{+})$ # 4. $D \frac{d}{dr} \phi(r) = |_{\mathbf{R}_{-}} = \hat{D} \frac{d}{dr} \phi(r) |_{\mathbf{R}_{+}}$
(3.59)

Appliying the boundary condition #1 by taking the limit of Eq. (3.57) as $r\rightarrow 0$, we see that the flux will remain finite only if $C_2=-C_1$. Using the definition of the hyperbolic sine, *Sinh*, then Eq. (3.57) reduces to

$$\phi(r) = \frac{2A}{r} \sinh(r/L) + \frac{S}{\sum_{a}} \quad 0 \le r < R \tag{3.60}$$

We next apply condition #2 to Eq. (3.58): Since the first term becomes infinite, but the second vanishes at $r \rightarrow \infty$, the condition is satisfied if A' = 0:

$$\phi(r) = \frac{C'}{r} e^{-r/L} \quad R < r \le \infty$$
(3.61)

At last we apply interface boundary conditions #3 and #4 the remaining arbitrary coefficients:

$$\frac{2A}{R}\sinh(R/L) + \frac{S}{\sum_{a}} = \frac{C'}{R}e^{-R/\hat{L}}$$
(3.62)

and

$$2DA\left[\frac{1}{RL}\cosh(R/L) - \frac{1}{R^2}\sinh(R/L)\right] = -\hat{D}C'(\frac{1}{R\hat{L}} + \frac{1}{R^2})e^{-R/\hat{L}}$$
(3.63)

When we solve Eq (3.62), C' becomes;

$$C' = \left(\frac{2A}{R}\sinh(R/L) + \frac{S}{\sum_{a}}\right) \operatorname{Re}^{R/\bar{L}}$$
(3.64)

Putting this into Eq. (3.63) we obtain the coefficient A as following

$$A = \frac{\frac{SR}{\sum_{a} \sinh(R/L)}}{2D(\frac{1}{L} \coth(R/L) - \frac{1}{R}) + 2\frac{\hat{D}}{R} \left(\frac{1}{\hat{L}} + \frac{1}{R}\right)}$$
(3.65)

Substituting A into Eq. (3.60), the result in the solution is found as

$$\phi(r) = \frac{2}{r} \sinh(r/L) \left(\frac{\frac{SR}{\sum_{a} \sinh(R/L)}}{2D\left(\frac{1}{L} \coth(R/L) - \frac{1}{R}\right) + 2\frac{\hat{D}}{R}\left(\frac{1}{L} + \frac{1}{R}\right)} \right) + \frac{S}{\sum_{a}} \qquad 0 \le r < R$$
(3.66)

And finally one obtains

$$\phi(r) = \frac{S}{\sum_{a}} \left(1 + \frac{R\sin(r/L)}{r\sinh(R/L)} \frac{1}{D\left(\frac{1}{L}\coth(R/L) - \frac{1}{R}\right) + \frac{\hat{D}}{R}\left(\frac{1}{\hat{L}} + \frac{1}{R}\right)} \right)$$
(3.67)

If we combine all the constans together

$$C'' = \left[1 + \frac{D}{\hat{D}} \frac{(R/L) \coth(R/L) - 1}{(R/\hat{L}) + 1}\right]^{-1}$$
(3.68)

The flux becomes

$$\phi(r) = \left[1 - \frac{R}{r} \frac{\sinh(r/L)}{\sinh(R/L)}\right] \frac{S}{\sum_{a}} \qquad 0 \le r < R \tag{3.69}$$

and one can write [2]

$$\phi(r) = (1 - C'') \frac{S}{\sum_{a}} \frac{R}{r} e^{\left[-(r-R)/\tilde{L}\right]} \qquad R < r \le \infty$$
(3.70)

CHAPTER 4

SOLUTION OF DIFFUSION EQUATION FOR MULTIPLYING SYSTEMS

In this Chapter we consider that our system has now fissionable material which is called "multiplying system". The solution of steady-state one-group diffusion equation for bare systems with fissionable materials in certain geometries is studied.

4.1 CRITICALITY ASSEMBLIES FOR SPHERE

In this system it is assumed to have fissionable material in the medium so $v\sum_f > 0$. Therefore, the diffusion equation that we represent into Eq. (3.19) is now defined by

$$\nabla^2 \phi - \frac{1}{L^2} \phi = -\frac{s}{D} - \frac{1}{L^2} k_{\infty} \phi$$

The Laplacian operator for spherical coordinates gives

$$-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\phi(r) + \frac{1}{L^2}(1-k_\infty)\phi(r) = \frac{S}{D}$$
(4.1)

To solve the non-homogeneous differential equation, homogeneous and particular solutions must firstly be solved for the general solution

$$\phi_g(r) = \phi_p(r) + \phi_h(r) \tag{4.2}$$

The particular solution goes to constant the derivation term vanishes and we have

$$\phi_p = \frac{S}{(1 - k_\infty) \sum_a} \tag{4.3}$$

The homogeneous solution satisfy

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\phi_h(r) - \frac{1}{L^2}(1-k_\infty)\phi_h(r) = 0$$
(4.4)

Using the function

$$\phi_h(r) = \frac{1}{r} \psi(r) \tag{4.5}$$

Eq. (4.4) is simplified as

$$\frac{d}{dr^2}\psi(r) - \frac{1}{L^2}(1 - k_{\infty})\psi(r) = 0$$
(4.6)

The form of the solution depends on k_∞ parameter: $k_\infty\!\!<\!\!1$ or $k_\infty\!\!>\!\!1.$

4.1.1 Subcritical Assemblies for Sphere

Firstly, we consider k_{∞} <1 condition to obtain the solution of the equation that we solved in preceding section. It is known that the solution is

$$\psi(r) = C \exp(\kappa r) \tag{4.7}$$

where $\kappa^2 = \frac{1}{L^2} (1 - k_{\infty})$ or equivalently

$$\kappa = \pm \frac{1}{L} \sqrt{1 - k_{\infty}} \tag{4.8}$$

Thus, one gets

$$\frac{d^2}{dr^2}\psi(r) = C\kappa^2 \exp(\kappa r)$$
(4.9)

Solution of Eq. (4.9) is now written as

$$\psi(r) = C_1 \exp(L^{-1}\sqrt{1-k_{\infty}}r) + C_2 \exp(-L^{-1}\sqrt{1-k_{\infty}}r)$$
(4.10)

Inserting this expression into Eqn. (4.5) and combining the result with Eqns. (4.2) and (4.3) we obtain the flux function in its general form as

$$\phi(r) = \frac{C_1}{r} \exp(L^{-1}\sqrt{1-k_\infty}r) + \frac{C_2}{r} \exp(-L^{-1}\sqrt{1-k_\infty}r) + \frac{S}{(1-k_\infty)\Sigma_a}$$
(4.11)

Then we apply the boundary conditions to obtain the constant. We can achieve condition that $\phi(0)$ must be finite only by requiring the two exponential terms to cancel exactly when r=0 thus we take $C_2 = -C_1$ then with the definition of the sinh(x) = $1/2(e^x - e^{-x})$, it becomes

$$\phi(r) = \frac{2C_1}{r} \sinh(L^{-1}\sqrt{1-k_{\infty}}r) + \frac{S}{(1-k_{\infty})\Sigma_a}$$
(4.12)

The second boundary condition is to be the extrapolated radius of the sphere $\phi(\tilde{R}) = 0$ and then Eq. (4.12) is now written as

$$0 = \frac{2C_1}{\tilde{R}} \sinh(L^{-1}\sqrt{1-k_{\infty}}\tilde{R}) + \frac{S}{(1-k_{\infty})\Sigma_a}$$
(4.13)

Solving for C_1 and inserting the result into Eq. (4.12) we find the flux for subcritical systems

$$\phi(r) = \frac{S}{(1 - k_{\infty})\sum_{a}} \left[1 - \frac{\tilde{R}}{r} \frac{\sinh(L^{-1}\sqrt{1 - k_{\infty}}r)}{\sinh(L^{-1}\sqrt{1 - k_{\infty}}\tilde{R})} \right]$$
(4.14)

4.1.2 Supercritical Assemblies for Sphere

Now we solve the diffusion equation for supercritical systems, that is, $k_{\infty} > 1$. For this purpose we may write same equations up to obtaining the general solution because we consider again same medium for supercritical systems so that diffusion equation remain same. That means, Eqn. (4.6) can be applied for general solution. However, the general solution takes a different form. This is most easily seen by noting that for $k_{\infty} > 1$ the second term of Eqn. (4.6) is now positive:

$$\frac{d}{dr^2}\psi(r) + \frac{1}{L^2}(k_{\infty} - 1)\psi(r) = 0$$
(4.15)

The general solution of this form differential equation becomes;

$$\psi(r) = C_1 \sin(L^{-1}\sqrt{k_{\infty} - 1}r) + C_2 \cos(L^{-1}\sqrt{k_{\infty} - 1}r)$$
(4.16)

Similarly to the $k_{\infty} < 1$ case, we insert this expression into Eqn. (4.5) and combine the result with Eqn. (4.2) and (4.3) to obtain the flux distribution

$$\phi(r) = \frac{C_1}{r} \sin(L^{-1}\sqrt{k_{\infty} - 1}r) + \frac{C_2}{r} \cos(L^{-1}\sqrt{k_{\infty} - 1}r) - \frac{S}{(k_{\infty} - 1)\Sigma_a}$$
(4.17)

One can apply the same boundary conditions as in the subcritical case: At the origin, $\phi(0)$ must be finite. Therefore, the second term becomes infinite unless we set C₂=0. Because $\cos(0)=1$ the first becomes finite since $\lim_{r\to 0} r^{-1} \sin(L^{-1}\sqrt{k_{\infty}-1}r) = L^{-1}\sqrt{k_{\infty}-1}$. If $\sin(Br)=n\pi$ at r=0, this becomes zero for critically condition and n takes the first value: n=1. Then, the term B is called *geometric buckling* that means $B_g = \pi/r$ and $B_m = L^{-1}\sqrt{k_{\infty}-1}$ in which B_m is *material buckling* depending on the material properties of the material composition of the reactor system.

Consequently

$$\phi(r) = \frac{C_1}{r} \sin(L^{-1}\sqrt{k_{\infty} - 1}r) - \frac{S}{(k_{\infty} - 1)\sum_a}$$
(4.18)

One can determine the constant C_1 by requiring using the boundary condition of $\phi(\tilde{R}) = 0$. Finally one obtains

$$\phi(r) = \frac{S}{(k_{\infty} - 1)\sum_{a}} \left[\frac{\tilde{R}}{r} \frac{\sin(L^{-1}\sqrt{k_{\infty} - 1}r)}{\sin(L^{-1}\sqrt{k_{\infty} - 1}\tilde{R})} - 1 \right]$$
(4.19)

This is the flux equation for the supercritical-spherical system [2, 3].

4.2 CRITICAL ASSEMBLIES FOR DIFFERENT GEOMETRIES

The criticality conditions for k=1 in different geometries with finite size are determined in the following sections. Three distinct geometries are considered and numerical results for bare systems with multiplying media are presented.

4.2.1 The Slab Reactor

Consider a bare reactor for critically condition consisting of an infinite bare slab of thickness *a* as shown in Figure 4.1. The reactor equation in this case becomes;

$$\frac{d^2\phi}{dx^2} + B^2\phi = 0 \tag{4.20}$$

where x is the distance from the center to the slab. The solution of this form of diffusion equation we know from the previous section;

$$\phi(x) = A\cos(Bx) + C\sin(Bx) \tag{4.21}$$



Figure 4.1: Slab reactor

To determine the two arbitrary constant boundary conditions must be applied. The first one is flux vanishes at the extrapolated faces of the slab, that is, at $x=-\tilde{a}/2$ where $\tilde{a}=a+2d$. Then the boundary condition becomes;

$$\phi(\frac{\tilde{a}}{2}) = \phi(-\frac{\tilde{a}}{2}) = 0 \tag{4.22}$$

It may also be noted that, because of the symmetry of the problem, there can be no net flow of neutrons at the center of the slab. Since the neutron current density is proportional to the derivative of ϕ , this means that

$$\frac{d\phi}{dx} = 0 \tag{4.23}$$

at x=0. The condition given by Eqn. (4.23) is equivalent to requiring that ϕ be an even function;

$$\phi(-x) = \phi(x) \tag{4.24}$$

and has a continuous derivative within the reactor. In the general solution A and C are constant to be determined. Placing the derivative of Eqn. (4.21) equal to zero at x=0 gives immediately C=0 reduces to

$$\phi(x) = A\cos Bx \tag{4.25}$$

Next, introducing the boundary condition given by Eqn. (4.22) gives;

$$\phi(\frac{\tilde{a}}{2}) = A\cos(\frac{B\tilde{a}}{2}) = 0 \tag{4.26}$$

This equation is satisfied both taking A=0, which leads to the trivial solution $\phi(x)=0$ and by requiring that

$$\cos(\frac{B\tilde{a}}{2}) = 0 \tag{4.27}$$

Eq. (4.27) is satisfied when

$$B_n = \frac{n\pi}{\tilde{a}} \tag{4.28}$$

and for integer values of "n" the critically condition is satisfied. Finally one obtains [1, 3]

$$\phi(x) = A\cos(\frac{\pi x}{\tilde{a}}) \tag{4.29}$$

To determine the valu of *A*, the calculation of total reactor power by fissions per cm³/sec, that is $\sum_{f} \phi(x)$ at the point *x*, and by using the recoverable energy is E_R joules per fission is obtained. The total power per unit area of the slab, in Watts/cm²:

$$P = E_R \sum_f \int_{-a/2}^{a/2} \phi(x) dx$$
 (4.30)

Substituting the flux equation Eq.(4.29) into Eq. (4.30);

$$P = E_R \sum_f \int_{-a/2}^{a/2} A\cos(\frac{\pi x}{\tilde{a}}) dx$$
(4.31)

After performing the integration the result becomes;

$$P = \frac{2\tilde{a}E_{R}\sum_{f}A\sin\left(\frac{\pi a}{2\tilde{a}}\right)}{\pi}$$
(4.32)

The unknown parameter A is now found to be

$$A = \frac{\pi P}{2\tilde{a}E_R \sum_f \sin\left(\frac{\pi a}{2\tilde{a}}\right)}$$
(4.33)

Replacing A value in the flux function for the slab in Eq.(4.29), one gets

$$\phi(x) = \frac{\pi P}{2\tilde{a}E_R \sum_f \sin\left(\frac{\pi a}{2\tilde{a}}\right)} \cos\left(\frac{\pi x}{\tilde{a}}\right)$$
(4.34)

4.2.2 Sphere

Consider a critical spherical reactor with radius R. The steady-state diffusion equation in spherical coordinates is now written as;

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d\phi}{dr} + B^2\phi = 0$$
(4.35)

By substituting $\phi = \omega/r$ into Eq. (4.35) one can obtain the general solution as

$$\phi(r) = A \frac{\sin BR}{r} + C \frac{\cos BR}{r} \tag{4.36}$$

where A and C are constants. As the first condition, when the r goes to zero, flux must be finite thus the second term becomes infinite. So C must be equal to zero. Hence the flux becomes

$$\phi(r) = A \frac{\sin(Br)}{r} \tag{4.37}$$

For the second boundary condition, $\phi(\tilde{R}) = 0$, it is yielded by taking *B* to be any one of the eigenvalues;

$$B_n = \frac{n\pi}{\tilde{R}} \tag{4.38}$$

where again n is an integer and the first value is relevant for a critical reactor. Thus the buckling parameter is found to be

$$B_1^2 = \left(\frac{\pi}{\tilde{R}}\right)^2 \tag{4.39}$$

Therefore, the flux function is written as

$$\phi(r) = A \frac{\sin(\pi r / \tilde{R})}{r}$$
(4.40)

This flux equation for sphere has an unknown coefficient that is found samely in slab reactor by using the reactor power calculation. If we write the power equation;

$$P = E_R \sum_f \int \phi(r) dV \tag{4.41}$$

where dV is the volume element of the sphere so it can be written as $dV = 4\pi r^2 dr$, Now substituting the volume element and flux equations into the integral;

$$P = E_R \sum_f 4\pi A \int_0^R \frac{\sin(\pi r/\tilde{R})}{r} r^2 dr \qquad (4.42)$$

Now the integration is found as;

$$P = E_R \sum_f 4\pi A \frac{\tilde{R}}{\pi} \left(\sin\left(\frac{\pi R}{\tilde{R}}\right) \frac{\tilde{R}}{\pi} - R \cos\left(\frac{\pi R}{\tilde{R}}\right) \right)$$
(4.43)

If we write the A value in terms of other parameters, one gets

$$A = \frac{\pi P}{E_R \sum_f 4\pi \tilde{R} \left(\sin\left(\frac{\pi R}{\tilde{R}}\right) \frac{\tilde{R}}{\pi} - R \cos\left(\frac{\pi R}{\tilde{R}}\right) \right)}$$
(4.44)

After inserting the expression of A into the flux function in Eq.(4.40), one obtains

$$\phi(r) = \frac{\pi P}{E_R \sum_f 4\pi \tilde{R} \left(\sin\left(\frac{\pi R}{\tilde{R}}\right) \frac{\tilde{R}}{\pi} - R \cos\left(\frac{\pi R}{\tilde{R}}\right) \right)} \frac{\sin(\pi r / \tilde{R})}{r}$$
(4.45)

In the system if extrapolation distance, d, is small and ignored in the Eq.(4.45), so the flux of the sphere can be written as;

$$\phi(r) = \frac{P}{E_R \sum_f 4R^2} \frac{\sin(\pi r / \tilde{R})}{r}$$
(4.46)

Since the material buckling is related to the material composition and is defined as $B_m^2 = (k_\infty - 1)/L^2$ one can obtain a relation between the radius of the system and the material composition; $L^{-1}\sqrt{k_\infty - 1}$. Therefore, the critic radius and also the critic mass of bare spherical reactor is as following;

$$B_m^2 = B_g^2 \tag{4.47}$$

Then, one finds the critic radius of the sphere as

$$R = \frac{\pi L}{\sqrt{k_{\infty} - 1}} \tag{4.48}$$

The following data is used to calculate the critical size and the critic mass of the pure uranium-235 system for 1.0 MeV neutrons [10, 11, 12]: v = 2.42, $\sigma_f = 1.336 b$, $\sigma_s = 5.959 b$, $\sigma_c = 0.153 b$, $N = 0.048 \times 10^{24} a toms/cm^3$ and $\rho = 18.75 gr/cm^3$. Then one finds the critic radius as 10.53 cm and 1.99 cm extrapolated distance then dropping 8.55 cm and the critical mass is found 49.85 kg (nearly 50 kg) [13, 14, 15]. In Refs. [13, 14, 15], different methods have been applied to solve the steady-state neutron diffusion equation. In Ref. [13], OB-1 method includes consists of the Maxwellian averaged fission and absorption cross sections and the thermal values of *nubar* values. The method based on the square-fitting of the evaluated data values. Ref. [14] applies the F_N method to the one-group diffusion equation in spherical geometry. The method based on the integration of equally spaced intervals of
unknown flux function depending on the parameter c of which values are between 1 and 2. The method is particularly efficient if and only if the polynomials and the log functions are coefficients in the system of algebraic equations obtained in the process. Ref. [15] consists a relatively simple method to calculate the critical mass of fissionable istopes. It is based on three simplifications such that non-fission absorption of neutrons is ignored, the f neutrons are assumed only to be emitted along the radial direction and the all emitted neutrons are monoenergetic. It includes the series expansion of the flux function under these conditions.

Table 4.1 Neutron cross-sections for ²³⁵Uand ²³⁹Pu used in Ref. [16], for 2 MeV neutrons.

Material	$\sigma_{_f}$	$\sigma_{_s}$	$\sigma_{_c}$	$\sigma_{_a}$	$\sigma_{_T}$	υ
235 U	1.287	5.804	0.0593	1.346	7.150	2.42
239 Pu	1.947	5.245	0.00799	1.982	7.227	2.98

Table 4.2 The critic radius and critic mass values at 2MeV neutron cross-sections for ²³⁵U and ²³⁹Pu spheres from data library [16]

Motorial	Present Results		Ref [17]		Percent Error %	
Material	R	М	R	М	R	М
	(cm)	(kg)	(cm)	(kg)	(cm)	(kg)
235 U	8.61	49.72	8.92	50.7	3.47	1.93
239 Pu	4.88	9.64	4.99	10.321	2.20	6.59

Additionally, one can also calculate the critic radius and critic mass values for bare spheres ²³⁵U and ²³⁹Pu for 2MeV neutrons by using the updated data Library [16]

given in Table 4.1. The calculated results by using library cross-section data are represented in Table 4.2

Subtracting the extrapolated distance, that is, d=2.07 cm from the radius of the sphere, the critic radius of the sphere is found to be 8.61 cm and the corresponding critic mass is calculated as 49.72 kg. On the hand, the critic radius of the sphere with non-extrapolated radius is found as 10.68 cm and the corresponding critic mass is found as 94.91 kg. This result is compared with other geometries in the following sections. By applying the same procedure for a pure Pu²³⁹ spherical reactor core, the extrapolated radius is yielded as 6.85 cm then subtracting the extrapolation distance - that is d=1.97 cm- the non-extrapolated radius becomes 4.88 cm. Then, the corresponding critic mass for pure plutonium core is calculated as 9.64 kg (nearly 10 kg) [17, 18]

4.2.3 Infinite Cylinder

Now consider an infinite critical cylindrical reactor of radius R and infinite height Z in the diffusion equation we ignore Z because of infinite the flux depends on only r from the axis. With the Laplacian operator in cylindrical coordinates the reactor equation becomes

$$\frac{1}{r}\frac{d}{dr}r\frac{d\phi}{dr} + B^2\phi = 0 \tag{4.49}$$

When the differentiation in the first term is carried out

$$\frac{d^2\phi}{dr^2} + \frac{1}{r}\frac{d\phi}{dr} + B^2\phi = 0$$
(4.50)

This form recall us the Bessel differential equations as

$$\frac{d^2\phi}{dr^2} + \frac{1}{r}\frac{d\phi}{dr} + \left(B^2 - \frac{m^2}{r^2}\right)\phi = 0$$
(4.51)

where m is an arbitrary constant. When we compare Eqn. (4.50) with (4.51) it is shown that m is equal to zero. So the general solution can be written as

$$\phi = AJ_0(Br) + CY_0(Br)$$
(4.52)

where A and C are constants. The functions assigned as $J_m(Br)$ and $Y_m(Br)$ are called ordinary Bessel functions of the first and second kind, respectively[19, 20]. The functions $J_0(x)$ and $Y_0(x)$ shown in Figure 4.2 gives us $Y_0(x)$ is infinite at x=0 while $J_0(0)=2.405$. Therefore, C must be taken to be zero, due to ϕ remaining finite within the reactor. Thus Eq. (4.50) reduces to form of

$$\phi(r) = AJ_0(Br) \tag{4.53}$$

Applying the boundary condition for $\phi(\tilde{R}) = 0$, one finds

$$\phi(\tilde{R}) = AJ_0(B\tilde{R}) = 0 \tag{4.54}$$

The function J_0 is equal to zero at a number of values of x so that $J_0(x_n)=0$. So, Eq. (4.52) is satisfied with providing *B* defined as

$$B_n = \frac{x_n}{\tilde{R}} \tag{4.55}$$



Figure 4.2 Ordinary and modified Bessel functions

which are the eigenvalues of the problem. As explained below, only the first eigenvalue is relevant for the criticality condition that means n = 1. Therefore,

$$B_{_{1}}^{2} = \left(\frac{x_{_{1}}}{\tilde{R}}\right)^{2} = \left(\frac{2.405}{\tilde{R}}\right)^{2}$$
(4.56)

Then the flux equation becomes;

$$\phi(r) = AJ_0\left(\frac{2.405r}{\tilde{R}}\right) \tag{4.57}$$

To define A, the same procedure is applied, if we write the flux Eq. (4.57) and cylinder volume element $dV = 2\pi r dr$ into the power equation by considering the d is small, so it becomes

$$P = 2\pi E_R \sum_f A \int_0^R J_0 \left(\frac{2.405r}{R}\right) r dr$$
 (4.58)

The integral is solved by using the Bessel Function integral rule that is;

$$\int J_0(x) x dx = x J_1(x) \tag{4.59}$$

If we apply this rule the power is found as;

$$P = \frac{2\pi E_R \sum_f AR^2 J_1(2.405)}{2.405}$$
(4.60)

If one uses the Bessel function properties of $J_1(2.405)$ is eqaul to 0.5202. If we put this number into equation and multiplying the constant

$$P = 1.359 E_R \sum_f A R^2 \tag{4.61}$$

Finally the flux equation for infinite cylinder becomes that;

$$\phi = \frac{0.735P}{E_R \sum_f R^2} J_0\left(\frac{2.405r}{R}\right)$$
(4.62)

The calculated critic radius of an infinite cylinder is presented in Table 4.3.

Boundary	R _c (cm)	R_{c} (cm)	Percent Error
Conditions	Ref. [10, 11, 12]	Present Result	%
Extrapolated distance	8.0589	8.0590	0.00124
Non-extrapolated distance	6.1863	6.1864	0.00162

Table 4.3 Critical radius for infinite cylinder, 1 MeV neutrons.

In Ref. [10,11, 12], the homotopy perturbation method that includes the change of variables and the series solution of the diffusion equation to obtain the numerical results.

4.2.4 Finite Cylinder

As another geometry, the cylinder with fi nite height and radius is examined. Therefore, the flux function now depends on r and z variables. The diffusion equation in cylindrical coordinates is written as

$$\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial\phi(r,z)}{\partial z} + \frac{\partial^2\phi(r,z)}{\partial z^2} + B^2\phi(r,z) = 0$$
(4.63)

where the boundary conditions are given as $0 < \phi(r, z) < \infty$; $0 \le r \le \tilde{R}$ and $-\tilde{H}/2 \le z \le \tilde{H}/2$. To obtain the solution, separation of variables is defined as

$$\phi(r,z) = \psi(r)\chi(z) \tag{4.64}$$

Then one writes

$$\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial z}\left(\psi(r)\chi(z)\right) + \frac{\partial^2}{\partial z^2}\left(\psi(r)\chi(z)\right) + B^2\psi(r)\chi(z) = 0$$
(4.65)

Following the partial derivatives and then dividing the final equation by $\psi(r)\chi(z)$, one obtains

$$\frac{1}{\psi} \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial \psi}{\partial r} + \frac{1}{\chi} \frac{\partial^2 \chi}{\partial z^2} + B^2 = 0$$
(4.66)

This equation must be satisfied for any r or z combination; the first and second terms must be constants so the first part can be written as

$$\frac{1}{\psi r}\frac{d}{dr}r\frac{d}{dr}\psi + B_r^2 = 0 \tag{4.67}$$

where B_r is the Buckling parameter for the radial part. Eq. (4.65) is in the form of Bessel differential equation of the first-kind zero order and its solution, as we have found in Eq. (4.50), is given by

$$\psi(r) = AJ_0(B_r r) + CY_0(B_r r)$$
(4.68)

Applying the same boundary condition in infinite cylinder, then Y_0 term drops from the equation. We know the value of B_r from Eq. (4.53).

For the *z*-dependent part we have

$$\frac{d^2\chi}{dz^2} + B_z^2 \chi = 0$$
 (4.69)

The solution of this form of differential equation is given by

$$\chi(z) = A'\cos(B_z z) + C'\sin(B_z z)$$
(4.70)

This equation is the same as for the infinite slab reactor. Using the boundary condition for the height, $-\tilde{H}/2 \le z \le \tilde{H}/2$ and $\phi(\tilde{H}/2) = 0$, one sets C' = 0 for the acceptable solution for the flux function that must be symmetric about the origin:

$$\chi(z) = A' \cos(B_z z) \tag{4.71}$$

The total buckling B^2 is;

$$B^2 = B_r^2 + B_z^2 \tag{4.72}$$

where B_r is the same as infinite cylinder for critically condition given in Eqs. (4.52) to (4.54) and B_z is found as similar as infinite slab given in Eqs. (4.26) to (4.29). So, one can write

$$B_z^2 = \left(\frac{\pi}{\tilde{H}}\right)^2, \quad B_r^2 = \left(\frac{2.405}{\tilde{R}}\right)^2 \tag{4.73}$$

The general solution is obtained with the required boundary conditions as

$$\phi(r,z) = AJ_0\left(\frac{2.405r}{\tilde{R}}\right)\cos(\frac{\pi z}{\tilde{H}})$$
(4.74)

Samely, to determine *A* if we put the finite cylinder flux into total power equation, it becomes;

$$P = E_R \sum_f \int_0^R \int_{-H/2}^{H/2} A J_0 \left(\frac{2.405r}{\tilde{R}}\right) \cos(\frac{\pi z}{\tilde{H}}) 2\pi r dr dz$$

$$\tag{4.75}$$

where the radial part of the integral result from the infinite cylinder solution is known. When the axial part of the integral is solved, we get;

$$P = E_R \sum_{f} A2\pi \frac{R^2}{2.405} J_1(2.405) \int_{-H/2}^{H/2} \cos(\frac{\pi z}{\tilde{H}}) dz$$
(4.76)

Solving for the axial part one gets

$$P = E_R \sum_f A4\pi \frac{R^2}{2.405} J_1(2.405) \frac{H}{\pi}$$
(4.77)

Solving for A one obtains

$$A = \frac{P2.405\pi}{E_R \sum_f 4\pi R^2 H J_1(2.405)} = \frac{3.63P}{V E_R \sum_f}$$
(4.78)

Replacing the value of A into the finite cylinder flux Eq.(4.74) one obtains

$$\phi(r,z) = \frac{3.63P}{VE_R \sum_f} J_0\left(\frac{2.405r}{\tilde{R}}\right) \cos(\frac{\pi z}{\tilde{H}})$$
(4.79)

where $\tilde{R} = R + d$ and $\tilde{H} = H + 2d$. Numerical applications are presented in Table 4.4, 4.5 - 4.6 for pure 235U and 239Pu fuel elements [13, 14]. A set of chosen critical height values corresponding critical radii of a finite cylinder calculated list is tabulated in Table 4.4 with corresponding reference values.

As seen in Table 4.4, the critic radius of a finite cylinder reduces to a certain value about 6.186 cm for 1 MeV neutrons as the height of the cylinder is increased. It means that the system behaves like an infinite cylinder of which radius is also given in Table 4.3. There is a correspondence between our results.

In Table 4.5, we present the critic radius and the critic mass of the finite cylinder for 235 U, for 2MeV neutrons. As the height of the cylinder is increased, it is observed that the critic radius is decreased. It is observed that the mass reaches at its minimum value at a certain height and radius of the cylinder. When the height is 18.32 cm and the corresponding radius is 7.9705 cm with the non-extrapolated distance, then the minimum critic mass is found to be 52.58963 kg.

We also present the numerical results for ²³⁹Pu, for 2MeV neutrons in Table 4.6.

	\tilde{R} cm	R cm	$ ilde{R}$ cm	R cm	\tilde{R} cm R cm
Ĥ cm	[Ref 9]	[Ref 9]	Present	Present Results	Percent Error %
			Kesuits	Results	
10.529	665.253	663.381	665.126258	663.253658	0.0200 0.0192
10.530	439.235	437.362	439.195063	437.322463	0.0090 0.0091
11.000	27.817	25.9445	27.816750	25.944150	0.0001 0.0015
12.000	16.7953	14.9227	16.795064	14.922464	0.0014 0.0013
13.000	13.7383	11.8657	13.738167	11.865567	0.0010 0.0017
14.000	12.2267	10.3541	12.226542	10.353942	0.9000 0.0019
15.000	11.3144	9.44178	11.314240	9.441640	0.0018 0.0015
20.000	9.47880	7.60620	9.478681	7.606081	0.0020 0.0015
30.000	8.60656	6.73396	8.606450	6.733850	0.0018 0.0016
40.000	8.35371	6.48111	8.353609	6.481009	0.0012 0.0015
50.000	8.24399	6.37139	8.243887	6.371287	0.0012 0.0016
100.000	8.10420	6.23160	8.104098	6.231498	0.0013 0.0016
200.000	8.07035	6.19775	8.070248	6.197648	0.0013 0.0016
400.000	8.06195	6.18935	8.061852	6.189252	0.0012 0.0015
600.000	8.06040	6.18780	8.060300	6.187700	0.0012 0.0016
800.000	8.05986	6.18726	8.059757	6.187157	0.0013 0.0016
1000.000	8.05961	6.18701	8.059506	6.186906	0.0013 0.0016

Table 4.4 Comparison of chosen heights and the corresponding critical radii with extrapolated distance and non-extrapolated distance for bare finite cylinder of ²³⁵U.

$ ilde{H}$ cm	Н ст	\tilde{R} cm	R cm	M kg
10.67	6.5200	651.6670	649.590	160764.1000
10.70	6.5500	107.6560	105.580	4219.71100
11.00	6.8500	33.5550	31.4780	396.61300
16.00	11.8465	10.9601	8.8833	54.62643
18.00	13.8465	10.1411	8.0643	52.61846
18.31	14.1565	10.0501	7.9733	52.58968
18.32	14.1665	10.0472	7.9705	52.58963
18.33	14,1765	10.0445	7.9677	52,58964
10.00	1 11 7 00	1010110	112077	02100701
20	15.85	9.6560	7.5790	53.07400
50	45.85	8.3600	6.2830	105.66200
100	95.85	8.2140	6.1370	210.4600
200	195.85	8.1790	6.1020	425.83900
400	395.85	8.1700	6.0930	857.88200
800	795.85	8.1680	6.0910	1725.32600
1000	995.85	8.1680	6.0910	2158.90700
1000	775.05	0.1000	0.0710	2130.90700

Table 4.5 Chosen heights and the corresponding critical radii and critical masses with extrapolated distance and non-extrapolated distance for ²³⁵U, for 2MeV neutrons.

\tilde{H} cm	Н ст	<i>Ã cm</i>	R cm	M kg
				C C
6.85	2.909	427.158	425.186	32713.723
6.86	2.916	112.089	110.116	2199.396
7.00	3.056	25.687	23,715	106 909
1100	21020	20.007	201110	1001/07
8.00	4.056	10.165	8.193	16.935
10.00	6.056	7.000	5.000	10.202
10.00	6.056	7.202	5.230	10.303
11.00	7.055240	6.705983	4.733603	9.8336
11.67	7.725240	6.480713	4.508333	9.766953
11 (0	7 7252 40	6 477707	4 505 417	0.7660.47
11.08	7.735240	0.4///9/	4.303417	9./0094/
11.69	7.745240	4.502512	6.474892	9.766965
11.70	7.755240	6.471998	4.499618	9.7670
15	11.056	5 897	3 924	10 5890
15	11.050	5.077	5.724	10.5070
20	16.056	5.583	3.611	13.0220
50	46.056	5.295	3.323	31.6340
100	96.056	5.258	3.285	64.4770
100	201020	0.200	0.200	0
200	196.056	5.248	3.276	130.8820
400	206.056	5.045	2.074	264.0750
400	396.036	5.246	3.274	264.0760
800	796.056	5.246	3.273	530.4570
1000	996.056	5.245	3.273	663.7290

Table 4.6 Chosen heights and the corresponding critical radii and critical masses with extrapolated distance and non-extrapolated distance for ²³⁹Pu, for 2MeV neutrons

4.2.5 Rectangular Parallel-piped

As a last example, we consider rectangular parallel piped system. The diffusion equation depends on the length of rectangular parallel piped a, b, c. Therefore, the diffusion equation

$$\nabla^2 \phi + B^2 \phi = 0 \tag{4.80}$$

with appropriate Laplacian operator in Cartesian coordinates is written as

$$\frac{d^2\phi}{dx^2} + \frac{d^2\phi}{dy^2} + \frac{d^2\phi}{dz^2} + B^2\phi = 0$$
(4.81)

Using the variable separation

$$\phi(x, y, z) = A(x)B(y)C(z) \tag{4.82}$$

one writes

$$\frac{d^2 A(x)B(y)C(z)}{dx^2} + \frac{d^2 A(x)B(y)C(z)}{dy^2} + \frac{d^2 A(x)B(y)C(z)}{dz^2} + B^2 A(x)B(y)C(z) = 0$$
(4.83)

Then three differential equations are obtained as following

$$\frac{d^{2}A(x)}{dx^{2}} + B_{x}^{2} = 0$$

$$\frac{d^{2}B(y)}{dy^{2}} + B_{y}^{2} = 0$$

$$\frac{d^{2}C(z)}{dz^{2}} + B_{z}^{2} = 0$$
(4.84)

Here the buckling is defined as

$$\frac{\tilde{a}}{2}B_x = n\frac{\pi}{2} \Longrightarrow B_x = \frac{n\pi}{\tilde{a}}$$
(4.90)

$$B^{2} = B_{x}^{2} + B_{y}^{2} + B_{z}^{2}$$
(4.85)

The solution of equations in Eq. (4.80) are found to be

$$A(x) = A' \sin(xB_x) + A'' \cos(xB_x)$$

$$B(y) = B' \sin(yB_y) + B'' \cos(yB_y)$$

$$C(z) = C' \sin(zB_z) + C'' \cos(zB_z)$$

(4.86)

For the boundary conditions when *a*, *b*, $c \rightarrow 0$, ϕ must be finite. So the first term in each solutions becomes zero. Then, one gets

$$\phi = A'' \cos(xB_x)B'' \cos(yB_y)C'' \cos(zB_z)$$
(4.87)

For any arbitrary constant, one can write Eq. (4.83) in the form of

$$\phi = K \cos(xB_x) \cos(yB_y) \cos(zB_z)$$
(4.88)

Applying the boundary conditions for each axis, one writes

$$\phi(\frac{\tilde{a}}{2}, y, z) = 0, \phi(x, \frac{\tilde{b}}{2}, z) = 0 \text{ and } \phi(x, y, \frac{\tilde{c}}{2}) = 0$$
(4.89)

Eq. (4.89) means that, buckling parameter for each side must provide the condition such as

From the critically condition we take a for the first value, and also the other has similar value so the Buckling becomes;

$$B^{2} = \left(\frac{\pi}{a}\right)^{2} + \left(\frac{\pi}{b}\right)^{2} + \left(\frac{\pi}{c}\right)^{2}$$
(4.91)

Finally the flux function is obtained as

$$\phi(x, y, z) = K \cos(\frac{\pi}{a} x) \cos(\frac{\pi}{b} y) \cos(\frac{\pi}{c} z)$$
(4.92)

Let define the unknown coefficient *K* by using the same procedure;

$$P = E_R \sum_{f} \int_{-a/2}^{a/2} \int_{-b/2}^{b/2} \int_{-c/2}^{c/2} K \cos(\frac{\pi}{a}x) \cos(\frac{\pi}{b}y) \cos(\frac{\pi}{c}z) dx dy dz$$
(4.93)

If we solve this integral the constant K is found as

$$K = \frac{\pi^3 P}{8abcE_R \Sigma_f} = \frac{3.87P}{VE_R \Sigma_f}$$
(4.94)

Now, after inserting the value of K into the flux of rectangular parallpiped this result is obtained

$$\phi(x, y, z) = \frac{3.87P}{VE_R \sum_f} \cos(\frac{\pi}{a} x) \cos(\frac{\pi}{b} y) \cos(\frac{\pi}{c} z)$$
(4.95)

In Table 4.7, the Buckling parameters and the neutron flux functions in different geometries are tabulated.

Geometry	Dimension	Buckling	Flux
Infinite slab	Thickness a	$\left(\frac{\pi}{a}\right)^2$	$A\cos\left(\frac{\pi x}{a}\right)$
Rectangular paralelpiped	a x b x c	$\left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{b}\right)^2 + \left(\frac{\pi}{c}\right)^2$	$K\cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi y}{b}\right)\cos\left(\frac{\pi z}{c}\right)$
Infinite cylinder	Radius R	$\left(\frac{2.405}{R}\right)^2$	$AJ_0\left(rac{2.405r}{R} ight)$
Finite cylinder	Radius R Height H	$\left(\frac{2.405}{R}\right)^2 + \left(\frac{\pi}{H}\right)^2$	$AJ_0\left(\frac{2.405r}{R}\right)\cos\left(\frac{\pi z}{H}\right)$
Sphere	Radius R	$\left(\frac{\pi}{R}\right)^2$	$A\frac{1}{r}\sin\left(\frac{\pi r}{R}\right)$

Table 4.7 Buckling and flux distributions in Bare systems for distinct geometries [1, 5]

CHAPTER 5

REFLECTED REACTORS

A reflector reduces the fraction of the neutrons leaking from the reactor, that is, they are reflected back into core [21]. A reflector's importance diminishes as the size of a reactor becomes larger. Neutron distribution equations within a uniform core remain valid for reflected reactors. To solve a reflected reactor system the same diffusion equation is used, however, the boundary conditions are different when the reflector is added, the core size is reduced. Now the axial and spherical reflector applications for two different reflector material combinations are considered in this Chapter.

5.1 AXIAL REFLECTOR

In a reflector there is no fissionable material so the diffusion equation becomes

$$\nabla^2 \phi - \frac{1}{L^2} \phi = 0 \tag{5.1}$$

where the diffusion length is the parameter of the reflector material. In cylindrical geometry the Laplacian operator takes the form as

$$\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}\phi + \frac{d^2}{dz^2}\phi - \frac{1}{L^2}\phi = 0$$
(5.2)

Now we separate variables

$$\phi(r,z) = \psi(r)\zeta(z) \tag{5.3}$$



Figure 5.1 Axial - Reflector

Then the result is divided by $\psi \zeta$ to yield

$$\frac{1}{\psi r}\frac{d}{dr}r\frac{d}{dr}\psi + \frac{1}{\zeta}\frac{d^2}{dz^2}\zeta - \frac{1}{L^2} = 0$$
(5.4)

From Eq. (4.65) one can

$$\frac{1}{\psi r}\frac{d}{dr}r\frac{d}{dr}\psi = -B_r^2$$
(5.4a)

and then rearranging Eq.(5.4) one obtains

$$\frac{1}{\zeta}\frac{d^2}{dz^2}\zeta - \left(B_r^2 + \frac{1}{L_r^2}\right) = 0$$
(5.4b)

where one can set a new parameter α^2 as

$$\alpha^2 = B_r^2 + \frac{1}{L_r^2} \,. \tag{5.5}$$

,

Thus, Eq. (5.4) reduces to

$$\frac{d^2}{dz^2}\zeta - \alpha^2 \zeta = 0 \tag{5.6}$$

The solution of this form for the axial reflector in Figure 5.1 is found as

$$\zeta(z) = A'' \exp(\alpha z) + C'' \exp(\alpha z)$$
(5.7)

We next add a reflector of height T to the top and bottom of the core. Adding the reflector reduces the height of the critical reactor from H to a yet to be determined value H'. Thus, the boundary conditions at top and bottom of the reflector removes the one of the arbitrary coefficients where $0 < \zeta(z) < \infty$ and $\left(-\frac{H'}{2} - T\right) \le z \le \left(\frac{H'}{2} + T\right)$:

$$\zeta\left(\frac{H'}{2}+T\right) = A''' \sinh\left(\alpha\left(\frac{H'}{2}+T\right)\right) + C''' \cosh\left(\alpha\left(\frac{H'}{2}+T\right)\right) = 0$$
(5.9)

Here the cosh term drops from the equation since it does not satisfy the boundary condition, C''' = 0, and the first term gives:

$$\zeta(z) = A''' \sinh(\alpha(H'/2 + T - z))$$
(5.10)

This equation represents the reflector flux and also we know the core flux equation from Eq. (4.68) as

$$\chi(z) = C' \cos(B'_z z) \tag{5.11}$$

in which B'_z is the buckling parameter for the reduced height of the core, H'. We now apply the interface boundary conditions at the core-reflector system: The continuity of the flux for the axial functions at the interface is

$$\chi(H'/2) = \zeta(H'/2)$$
(5.12)

which is

$$C'\cos(B_z z) = A'''\sinh(\alpha T)$$
(5.13)

and the current functions at the interface is

$$D_c \left. \frac{d}{dz} \chi(z) \right|_{H'/2} = D_r \left. \frac{d}{dz} \zeta(z) \right|_{H'/2}$$
(5.14)

then one gets

$$B'_z D_c C' \sin(B'_z H'/2) = \alpha D_r A''' \cosh(\alpha T)$$
(5.15)

When we divide Eq. (5.15) to Eq. (5.13) we obtain

$$B'_z D_c \tan(B'_z H'/2) = \alpha D_r \coth(\alpha T)$$
(5.16)

where D_c and D_r are diffusion coefficients of core and reflector, respectively. When T goes to infinity in Eq. (5.16), it means that the reflector has an infinite thickness and one finds $\operatorname{coth}(\infty) = 1$. So, Eq. (5.16) reduces to;

$$B'_{z} \tan(B'_{z}H'/2) = \alpha D_{r}/D_{c}$$
 (5.17)

Solving for H', one obtains

$$H' = \frac{2}{B'_z} \tan^{-1} \left(\alpha \frac{D_r}{B'_z D_c} \right)$$
(5.18)

This is the critic height of the finite cylinder with reflector Ref. [2]

T(cm)	$H_{exp}(cm)$	H _{non-exp}	M(kg)
0	18.320	14.167	52.589
1	16.415	12.262	45.519
2	14.965	10.812	40.135
4	13.556	9.402	34.902
6	13.156	9.003	33.420
8	13.055	8.901	33.043
10	13.030	8.876	32.950
20	13.021	8.868	32.919
50	13.021	8.868	32.919
100	13.021	8.868	32.919

Table 5.1 Axial Uranium core with Uranium reflector

T (cm)	$H_{exp}(cm)$	H _{non-exp}	M(kg)
0	18.320	14.167	52.589
1	16.342	12.188	45.245
2	14.937	10.783	40.031
4	13.761	9.607	35.664
6	13.497	9.343	34.684
8	13.443	9.290	34.486
10	13.433	9.279	34.446
20	13.430	9.276	34.436
50	13.430	9.276	34.436
100	13.430	9.276	34.436

Table 5.2 Axial Uranium core with Pu-239 Reflector

It is observed in Tables 5.1 and 5.2, the critic height of the bare reactor system reduces to a certain value when the thickness of the reflector is increased [10, 11, 12, 15, 22]. For the comparison at 2MeV neutrons, the first values in the first row are the critic height and the critic mass of the bare-finite-cylinder systems with pure 235U materials, given in Table 4.5.

5.2 SPHERICAL REFLECTOR

Consider a spherical reactor consisting of a radius R surrounded by a reflector having thickness T. Since there is no fissionable material in the reflector, the flux in this region satisfies the one group diffusion equation [1, 3]

$$\nabla^2 \phi_r - \frac{1}{L_r^2} \phi_r = 0$$
 (5.19)

The general solution of this equation is

$$\phi_r = A' \frac{\cosh(r/L_r)}{r} + C' \frac{\sinh(r/L_r)}{r}$$
(5.20)

where A' and C' are constants. Applying the condition for the vanishing of the flux ϕ_r at r = R + T where T is the thickness of the reflector.

$$A' \frac{\cosh(\frac{R+T}{L_r})}{r} = -C' \frac{\sinh(\frac{R+T}{L_r})}{r}$$
(5.21)

Considering C' from the Eq. (5.21), one gets

$$C' = -\frac{A'\cosh(\frac{R+T}{L_r})}{\sinh(\frac{R+T}{L_r})} = -A'\coth(\frac{R+T}{L_r})$$
(5.22)

If C' is substituted into flux Eq. (5.20) then one obtains

$$\phi_r = \frac{A'}{r\sinh(\frac{R+T}{L_r})} \left(\sinh(\frac{R+T}{L_r})\cosh(\frac{r}{L_r}) - \cosh(\frac{R+T}{L_r})\sinh(\frac{r}{L_r}) \right)$$
(5.23)

Rearranging Eq. (5.23), one obtains the flux function as

$$\phi_r = \frac{A'}{r\sinh(\frac{R+T}{L_r})}\sinh(\frac{R+T-r}{L_r})$$
(5.24)

Previously the solution in the core has known from solution of spherical bare reactor that is

$$\phi_c = A \frac{\sin(Br)}{r} \tag{5.25}$$

The functions ϕ_c and ϕ_r must be also satisfied at the interface boundary conditions: These conditions are

$$\phi_c(R') = \phi_r(R') \tag{5.26}$$

Appliying the boundary condition one finds

$$A\frac{\sin(BR)}{R} = \frac{A'}{R\sinh(\frac{R+T}{L_r})}\sinh(\frac{T}{L_r})$$
(5.27)

and using the definition of current function at the boundary one gets

$$D_c \left. \frac{d}{dr} \phi_c(r) \right|_{R'} = D_r \left. \frac{d}{dr} \phi_r(r) \right|_{R'}$$
(5.27)

Substituting the relevant equations one writes

$$AD_{c}\left(\frac{B\cos(Br)}{r} - \frac{\sin(Br)}{r^{2}}\right) = D_{r}\frac{A'}{\sinh(\frac{R+T}{L_{r}})}\left(\frac{\cosh(\frac{R+T-r}{L_{r}})}{L_{r}r} + \frac{\sinh(\frac{R+T}{L_{r}})}{r^{2}}\right)$$
(5.28)

Dividing Eq. (5.28) by Eq. (5.7) one gets

$$-D_{c}\left(\frac{B\cot(BR)-1}{R}\right) = D_{r}\left(\frac{\coth(\frac{T}{L_{r}})}{L_{r}} + \frac{1}{R}\right)$$
(5.29)

After some arrangement, one can write a more convenient form as

$$\cot(BR) = \frac{1}{BR} \left(1 - \frac{D_r}{D_c} \right) - \frac{D_r}{D_c} \frac{1}{BL_r} \coth(\frac{T}{L_r})$$
(5.30)

This equation represents the relationship between the core radius of sphere and the reflector thickness. For an infinite reflector the Eq. (5.30) becomes

$$BR\cot(BR) - 1 = -\frac{D_r}{D_c} \left(\frac{R}{L_r} + 1\right)$$
(5.31)

This equation must be satisfied for the reactor to be critical. For example if the composition of the core is known, the material Buckling can be determined and then the core radius, R, can be calculated, or vice versa.

As it is seen in Table 5.3 and Table 5.4, the critic radius of spherical core, surrounded by a reflector of which thickness is gradually increased, decreases to a certain final value. The decrease in critical size of a core due to a reflector is expressed by a term called "*reflector savings*, δ " and given by

$$\delta = R_c - R \tag{5.32}$$

where R_c is the critical radius of the unreflected system [23]. For a spherical system, R_c is defined in Eq. (4.34) as B/π . A plot of the reflector savings derived from Eqs. (5.31) and (5.32) as a function of pure ²³⁵U reflector thickness for the pure ²³⁵U core is presented in Figure 5.2. It is observed that beyond a certain reflector thickness, further increase does not affect the reflector savings. Our result in Figure 5.2 is in consistent with Ref. [5].



Figure 5.2 Calculated reflector saving as a function of Uranium reflector thickness

As shown in Table (5.5), the spherical 235 U core-reflector calculation results have 3.4% error with the existing literature, Ref. [24]. It is also shown that 239 Pu core-reflector spherical system has 1.6% error with the numerical value proposed in Ref. [24].

Г (<i>cm</i>)	<i>R'</i> (<i>cm</i>)	M(kg)
0	10.68	49.72
1	9.733	34.97
2	8.998	25.84
4	8.222	18.03
6	7.941	15.71
8	7.841	14.92
10	7.805	14.65
20	7.785	14.49
30	7 785	14 49

Table 5.3: Pure ²³⁵U core surroundedwith pure ²³⁵U reflector for sphere.

Table 5.4: Pure ²³⁹Pu core surrounded with pure ²³⁹Pu reflector for sphere.

Table 5.5: Comparision of spherical reflector results with literature

T (cm)	Core-Reflector materials	Ref[24] M (kg)	Present Results M (kg)	Percent Error %
infinite	²³⁵ U- ²³⁵ U	15.00	14.49	3.4
infinite	²³⁹ Pu- ²³⁹ Pu	1.80	1.83	1.6

CHAPTER 6

CONCLUSION

In this thesis work, solution of the steady-state one-group diffusion equation for bare and reflected reactor systems in three distinct geometries has been worked out for the calculation of the critic size and critical mass. A relation between the material composition and the size of the geometry in question has been obtained by the eigenvalue, called *Buckling* parameter, of the diffusion equation. It is observed that there is a direct relation between the material Buckling, B_m , and the geometric Buckling, B_g . It is also observed that a reflector material reduces the critic size and mass of a system.

Firstly, the derivation of the steady-state one-group diffusion equation is studied by reviewing the neutron reactions. After determining the parameters in the equation, the critical mass values in three distinct geometries for pure ²³⁵U and ²³⁹Pu materials are obtained by solving the steady-state one-group diffusion equation for bare reactor systems for certain neutron energy in fast region.

Then, the diffusion equation is solved for systems with a reflector surrounding the core to reduce the critic size of the original system: It is observed that there is a reduction in the size of the active core if a reflector is added into the system. Although the core and reflector are assumed to be made of same materials, for simplicity in calculations, a reduction which is called as "*reflector savings*" is also observed in all geometries in our examples. It is seen that the critic dimension of the

active core decreases down to a certain value even the thickness of the reflector is increased.

The results obtained in this thesis study are in consistent with existing numerical results in the literature. The method used in this study is the direct solution of the diffusion equation without using any approach and relatively simple with respect to other methods, given throughout the text, for estimating the critical mass of a fissionable element in all distinct geometries to obtain the solution of the neutron diffusion function for mixture material compositions in the nuclear reactor systems.

Since the steady-state one-group diffusion equation is considered in three basic geometries in this work, it is thought that the study can be extended to two-group calculations for different core-reflector material compositions. One can consider the solution of the diffusion equation by the Monte-Carlo Method for N-Group calculations. It is also possible to study the reactor kinetics, which are time-dependent parameters, of a reactor system as a future work.

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APPENDICES

APPENDIX A

GRADIENT

The gradient of a function f is defined as the vector whose componenets are equal to the rates of change of f along the direction of the component. Thus,

grad
$$f = \frac{\partial f}{\partial s_1} \mathbf{a}_1 + \frac{\partial f}{\partial s_2} \mathbf{a}_2 + \frac{\partial f}{\partial s_3} \mathbf{a}_3$$

Where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are unit vectors normal to the coordinate surfaces. It follows that the components of the gradient in rectangular coordinates are;

$$grad_x f = \frac{\partial f}{\partial x}, \quad grad_y f = \frac{\partial f}{\partial y}, \quad grad_z f = \frac{\partial f}{\partial z}$$

In cylindrical coordinates are;

$$grad_r f = \frac{\partial f}{\partial r}, \ grad_{\mathcal{G}} f = \frac{1}{r} \frac{\partial f}{\partial \mathcal{G}}, \ grad_z f = \frac{\partial f}{\partial z}$$

In spherical coordinates;

$$grad_r f = \frac{\partial f}{\partial r}, \ grad_{\mathcal{G}} f = \frac{1}{r \frac{\partial f}{\partial \mathcal{G}}}, \ grad_{\varphi} f = \frac{1}{r \sin \mathcal{G}} \frac{\partial f}{\partial \varphi}$$

DIVERGENCE

The general formula for the divergence of a vector in curvilinear coordinates can be obtained by applying the divergence theorem to the infinitely small volume element $dV = ds_1s_2s_3$ According to this theorem; the integral of the normal component of a vector over a closed surface is equal to the integral of the divergence of the vector throughout the enclosed volume. In symbols,

$$\int_{A} \mathbf{F} \cdot \mathbf{n} \, d\mathbf{A} = \int_{V} \mathbf{div} \, \mathbf{F} \, \mathbf{dV}$$

Where \mathbf{n} is a unit vector. If V is infinitely small, the volume integral is simply

$$div\mathbf{F} dV = \int_{A} \mathbf{F} \cdot \mathbf{n} \, d\mathbf{A}$$

Carrying out the integral over the faces of dV,

$$\int_{A} \mathbf{F} \cdot \mathbf{n} \, d\mathbf{A} = \left[\left(F_1 ds_2 ds_3 \right)_{q_1 + dq_1} - \left(F_1 ds_2 ds_3 \right)_{q_1} \right] \\ + \left[\left(F_2 ds_1 ds_3 \right)_{q_2 + dq_2} - \left(F_2 ds_1 ds_3 \right)_{q_2} \right] \\ + \left[\left(F_3 ds_1 ds_2 \right)_{q_3 + dq_3} - \left(F_3 ds_1 ds_2 \right)_{q_3} \right]$$

The first bracket can be written as

$$\begin{bmatrix} \left(F_1 ds_2 ds_3\right)_{q_1 + dq_1} - \left(F_1 ds_2 ds_3\right)_{q_1} \end{bmatrix} = \frac{\partial}{\partial q_1} \left(F_1 ds_2 ds_3\right) dq_1$$
$$= \frac{\partial}{\partial q_1} \left(F_1 h_2 h_3\right) dq_1 dq_2 dq_3$$

Combining terms then gives

$$div \mathbf{F} dV = \left[\frac{\partial}{\partial q_1} (F_1 h_2 h_3) + \frac{\partial}{\partial q_2} (F_2 h_1 h_3) + \frac{\partial}{\partial q_3} (F_3 h_1 h_2)\right] dq_1 dq_2 dq_3$$

Dividing by dV becomes finally

$$div \mathbf{F} = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1} (F_1 h_2 h_3) + \frac{\partial}{\partial q_2} (F_2 h_1 h_3) + \frac{\partial}{\partial q_3} (F_3 h_1 h_2) \right]$$

Introducing the values of the h's in rectangular coordinates gives

$$div \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

In cylindrical coordinates;

$$div \mathbf{F} = \frac{1}{r} \frac{\partial}{\partial r} (rF_r) + \frac{1}{r} \frac{\partial F_g}{\partial g} + \frac{\partial F_z}{\partial z}$$

In spherical coordinates;

$$div \mathbf{F} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 F_r \right) + \frac{1}{r \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta F_\vartheta \right) + \frac{1}{r \sin \vartheta} \frac{\partial F_\varphi}{\partial \varphi}$$

LAPLACIAN

This operator is the divergence of the gradient of a scalar function. The component F_1 of the gradient is

$$F_1 = \frac{1}{h_1} \frac{\partial f}{\partial q_1},$$

With similar expressions for the other components. Inserting these components into the previous formula for the divergence gives for the Laplacian:

$$\nabla^2 f = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial f}{\partial q_1} \right) + \frac{\partial}{\partial q_2} \left(\frac{h_1 h_3}{h_2} \frac{\partial f}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left(\frac{h_1 h_2}{h_3} \right) \frac{\partial f}{\partial q_3} \right]$$

The symmetry of this formula should be noted. In view of his result, the Laplacian in rectangular coordinates is;

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

In cylindrical coordinates ;

$$\nabla^2 f = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2}$$

And in spherical coordinates;

$$\nabla^2 f = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial f}{\partial \vartheta} \right) + \frac{1}{r^2 \sin^2 \vartheta} \frac{\partial^2 f}{\partial \varphi^2}$$

APPENDIX B

THE LINEAR EXTRAPOLATION DISTANCE FOR PLANE SURFACE

At the boundary there is a net flow of neutrons in one direction. It is assumed that "near the boundary between a diffusion medium and a vacuum the neutron flux varies in such a manner that linear extrapolation would require the flux to vanish at a given distance beyond the boundary. According the diffusion theory based on; Fick's Law are given by;

$$J_{+}(x) = \frac{\phi}{4} - \frac{D}{2} \frac{d\phi}{dx} \quad and \quad J_{-}(x) = \frac{\phi}{4} + \frac{D}{2} \frac{d\phi}{dx}$$

These are the x-component of the current function through the x-axis. The current J is known from the Fick's Law and also the difference of these two components is agreement with the current vector. As a boundary condition at the medium-vacuum intersection, the current density to the -x-direction, $J_{-}(x)$, is zero that means no neutrons scattered back from the vacuum. Therefore, one writes

$$J_{-}(x) = \frac{\phi_0}{4} + \frac{D}{2} \frac{d\phi_0}{dx} = 0$$

then one gets

$$\frac{1}{\phi_0} \frac{d\phi_0}{dx} = -\frac{1}{2D}$$

where $D = \frac{\lambda_{tr}}{3}$. Thus, one writes

$$\frac{1}{\phi_0} \frac{d\phi_0}{dx} = -\frac{3}{2\lambda_{tr}}$$

On the other hand, one defines the slope of the function ϕ_0 by using the geometry given in Figure B.1 as

$$\frac{\phi_0}{d} = \tan(\alpha) = -\frac{d\phi}{dx}\Big|_{x=0}$$

then one obtains


Figure B.1 Extrapolation distance of neutron flux at plane surface between diffusion medium and vacuum.