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Tokyo Institute of Technology

Nuclear Reactor Theory

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COE-INES Textbook

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Preface

Most students who enter the Graduate School of the Tokyo Institute of Technology to major in nuclear engineering have not taken classes in nuclear engineering when they were undergraduates. With this in mind, this course "Nuclear Reactor Theory" is designed for students who are studying nuclear engineering for the first time.

This textbook is composed of two parts. Part 1 "Elements of Nuclear Reactor Theory" is composed of only elements but the main resource for the lecture of nuclear reactor theory, and should be studied as common knowledge. Much space is therefore devoted to the history of nuclear energy production and to nuclear physics, and the material focuses on the principles of energy production in nuclear reactors. However, considering the heavy workload of students, these subjects are presented concisely, allowing students to read quickly through this textbook.

However, it is not sufficient to read only this part to understand nuclear reactor theory. I have tried to prepare Part 2 in addition to Part 1. Part 2 "Reactor Analysis" is aimed to cover all areas of reactor physics and contains detailed descriptions. However, available time is not enough for writing all acquired contents. In another lecture "Nuclear Engineering Design Laboratory", many students are solving neutron diffusion equations. Therefore, I add only "Transport Equation and Diffusion Equation" and "Numerical Analysis of Diffusion Equation" in Part 2. The contents in this Part are intended for self-studying and there is more than lectured contents. Other topics such as basic mathematics and time-dependent problems will be added in the future.

Every week, I will present a problem to be solved in the lecture. These problems are included in this textbook. I hope they will help in understanding the subject.

I hope that this textbook will stimulate the interest of students in nuclear reactor theory and help them to master the topic within a short period of time.

Hiroshi Sekimoto
Tokyo
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(1-1) Introduction

(1-1-1) Nuclear Reactor Theory and Reactor Analysis

In Part 1 "Elements of Nuclear Reactor Theory", we study an overview of nuclear reactors and how nuclear energy is extracted from reactors. Here, nuclear energy means the energy released in nuclear fission. This occurs because of the absorption of neutrons by fissile material. Neutrons are released by nuclear fission, and since the number of neutrons released is sufficiently greater than 1, a chain reaction of nuclear fission can be established. This allows, in turn, for energy to be extracted from the process. The amount of extracted energy can be adjusted by controlling the number of neutrons. The higher the power density is raised, the greater the economic efficiency of the reactor. The energy is extracted usually as heat via the coolant circulating in the reactor core. Finding the most efficient way to extract the energy is a critical issue. The higher the coolant output temperature is raised, the greater the energy conversion efficiency of the reactor. Considerations of material temperature limits and other constraints make a uniform power density desirable. Ultimately, this means careful control of the neutron distribution. If there is an accident in a reactor system, the power output will run out of control. This situation is almost the same as an increase in the number of neutrons. Thus, the theory of nuclear reactors can be considered the study of the behavior of neutrons in a nuclear reactor. The behavior of neutrons in a nuclear reactor will be described in Part 2.1 "Transport Equation and Diffusion Equation", which is a basis of Part 2 "Reactor Analysis".

Note that the two terms used here, "nuclear reactor theory" and "reactor analysis", are used to mean nearly the same thing. The terms "reactor physics" is also sometimes used. This field addresses the neutron transport including changes of neutron characteristics. However, with the development of the analysis of nuclear reactors, especially light water reactors, this field has taken on many facets. The scope of this textbook is not limited to light water reactors, but is intended to summarize the general knowledge about nuclear reactors.

(1-1-2) Discovery of the Neutron, Nuclear Fission and Invention of the Nuclear Reactor

Technology generally progresses gradually by the accumulation of basic knowledge and technological developments. In contrast, nuclear engineering was born with the unexpected discovery of neutrons and nuclear fission, leading to a sudden development of the technology. Progress of nuclear physics and nuclear engineering is shown in Table 1.1 with some related topics.

The neutron was discovered by Chadwick in 1932. This particle had previously been observed by Irene and Frederic Joliot-Curie. However, they interpreted the particle as being a high energy γ-ray. Considering that the Joliot-Curies were excellent scientists and later received a Nobel Prize, it can be understood how difficult it was to predict the neutron at that time. The discovery of neutrons clarified the basic structure of the atomic nucleus (often referred to as simply the "nucleus"), which consists of protons and neutrons. At the same time, the discovery of neutrons provided an extremely effective technology for producing nuclear reactions. Since the nucleus is very small, it is necessary to bring reacting nuclei close to each other in order to cause a nuclear reaction. Since the nucleus has a positive charge, a very large amount of energy is required to bring the nuclei close enough so that a reaction can take place. However, the neutron has no electric charge; thus, it can easily be brought close to a nucleus. Fermi clarified the effectiveness of this method by carrying out numerous nuclear reactions using neutrons, for which he received a Nobel Prize, and discovered that many nuclei can easily react with neutrons if the neutrons are moderated.

Table 1.1   Progress in nuclear physics

1808   Dalton: Atomic theory
1876   Goldstein: Cathode rays
1891   Stoney: Prediction of electrons
1895   Roentgen: X-rays
  1896   Becquerel: Radioactivity
1897   Thomson: Cathode rays = electrons
  1898   Rutherford: α-rays and β-rays
1900   Planck: Quantum theory
1905   Einstein: Special relativity theory
  1911   Rutherford: Atomic model
  1912   Thomson: Isotope
      1914-1918   World War 1
  1919   Aston: Mass spectrometer
  1921   Harkins: Prediction of neutrons
  1930   Bothe: Be (α, ?)
  1932   Irene and Frederic Joliot-Curie: Be (α, γ)
          Chadwick: Neutron discovery
  1934   Fermi: Delayed neutrons
          Szilard: Chain reaction
      1939-1945   World War 2
  1939   **Hahn, Strassman, Meitner: Discovery of nuclear fission**
    1942   **Fermi: CP–1 made critical**
    1944   First plutonium production reactor made critical (Hanford, USA)
    1945   Test of atomic bomb (USA)
    1945   Natural uranium heavy water research reactor (ZEEP) made critical (Canada)
    1946   Fast reactor (Clementine) made critical (USA)
    1950   Swimming pool reactor (BSR) made critical (USA)
    1951   Experimental fast breeder reactor (EBR-1) made critical and generates power (USA)
    1953   Test of hydrogen bomb (USSR)
          "Atoms for Peace" Initiative (United Nations, USA)
    1954   Launch of the nuclear submarine "Nautilus" (USA)
          Graphite-moderated water-cooled power reactor (AM-1) generates power (USSR)

Nuclear fission was discovered by Hahn, Strassman, and Meitner in 1939. Fission should have taken place in Fermi's experiments. The fact that Fermi did not notice this reaction indicates that nuclear fission is an unpredictable phenomenon. In 1942, Fermi created a critical pile after learning about nuclear fission and achieved a chain reaction of nuclear fission. The output power of the reaction was close to nil, however, this can be considered the first nuclear reactor made by a human being.

Reflecting on this history, we can understand how the discovery of the neutron and nuclear fission was unexpected. We can also appreciate how fast a nuclear reactor was built once these discoveries were made. This is very similar to the case of X-rays, where several X-ray generators were put on the market in the year following the discovery of X-rays by Roentgen in 1895, and X-rays began to be used not only in the laboratory but also for practical applications such as for the treatment of cancer and for hair removal.

However, it is not the case that a nuclear reactor can be built simply by causing fissions by bombarding nuclei with neutrons. The following conditions have to be satisfied for nuclear fission reactions. (As it turned out, these conditions could be satisfied within one year after the discovery of nuclear fission.)

① Exoergic reaction
② Sustainable as a chain reaction
③ Controllable

Details of these conditions and the theory of nuclear reactors are explained in the following sections. Since Part I is designed to be a review, the subject is explained with as few equations as possible so that beginners can easily understand it.

It was obvious to the researchers of that time that a nuclear reaction can generate approximately one million times the energy of a chemical reaction. The above-mentioned first nuclear reactor was built by Fermi under a plutonium production project for atomic bombs. In a nuclear reactor, radioactive material is rapidly formed. Therefore, nuclear reactors have the following unique and difficult issues, which did not have to be considered for other power generators.

① Safety
② Waste
③ Nuclear proliferation

Solving these issues is a big problem and they will be touched on in this course.

The first nuclear reactor was built in the middle of World War II in the military research and development program known as the Manhattan Project. Its products were the atomic bombs using enriched uranium and plutonium. One of the reasons for this war was to secure energy sources. After the war, the energy problem remained a big issue. Thus, large-scale development of nuclear engineering was started in preparation for the exhaustion of fossil fuels.

Light-water reactors, which were put into practical use in nuclear submarines, were established in many countries. These reactors are not a solution to the energy problem, since they can utilize less than 1% of natural uranium. Fast reactors, on the other hand, can use almost 100% of natural uranium. However, after new energy resources were discovered and the depletion of resources became remote, the development of fast reactors, which were considered the solution to the energy problem at the time, met a world-wide setback. Now the problem of the global environment is at the fore, and nuclear engineering, which does not generate carbon dioxide, is being reconsidered. Although it will not be discussed in this course, it is important to keep this issue in the back of our minds.

Nuclear engineering is an excellent technology by which tremendous amounts of energy is generated from a small amount of fuel. In addition to power generation, numerous applications are expected in the future. As well as being used in energy generation, neutrons are expected to be widely used as a medium in nuclear reactions.

(1-2) Nuclear Structure and Nuclear Energy

(1-2-1) Elementary Particles and Fundamental Forces

Matter was once considered to be made simply of atoms. It was soon discovered that atoms are made of elementary particles. Furthermore, it turned out that some elementary particles have a further fine structure. At present, the most fundamental particles that constitute material are those shown in Figure 1.1, classified into two main kinds, depending upon whether they are matter particles or force-carrier particles.

Fundamental elementary particles
- Matter particles (fermions)
  - Quark
  - Lepton
- Force-carrier particles / Gauge particles (bosons)
  - Graviton
  - Photon
  - Weak boson
  - Gluon
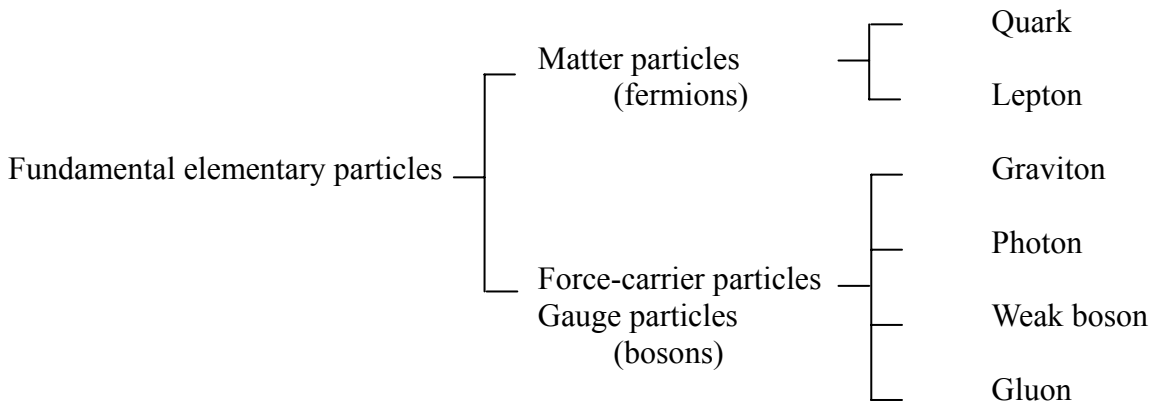
Figure 1.1 Elementary particles

Table 1.2   Quarks and Leptons

	charge			
quark	2/3	u (up)	c (charm)	t (top)
	- 1/3	d (down)	s (strange)	b (bottom)
lepton	0	ν_e	ν_μ	ν_τ
	−1	e (electron)	μ (muon)	τ (tau)

Table 1.3   The four kinds of forces and gauge particles

Interaction	Gauge particle	Range of force
Gravitational interaction	Graviton	∞
Weak interaction	Weak boson (W^+, W^-, Z^0)	$\gtrsim 10^{-18}$ m
Electromagnetic interaction	Photon	∞
Strong interaction	Gluon	$\gtrsim 10^{-15}$ m

Matter particles, referred to as "fermions", have 1/2 spin, obey Fermi-Dirac statistics, and obey the Pauli exclusion principle. These particles are further classified into quarks, which constitute hadrons (elementary particles that exhibit strong interaction, such as the proton, neutron, and pion (π meson)) and leptons (which do not exhibit strong interaction). Specific members of these sub-classifications are shown in Table 1.2. Each group contains six members and they are symmetrical.

At extremely high temperatures, such as at the beginning of the universe, there is supposedly one force. As temperature decreases, this force is gradually differentiated into the present four interactions: gravitational, weak, electromagnetic, and strong interactions. As shown in Table 1.3, these interactions are due to respective exchange particles (referred to as gauge particles). These particles, referred to as "bosons", have spin 1 and obey Bose-Einstein statistics. The mass of each of these particles is considered to be zero except for that of the weak boson. The electric charge of these particles except $W^{+/-}$ is zero. The gravitational and electromagnetic interactions are long-range forces, and their change is proportional to $1/r$, where r is the separation. The weak and strong interactions are short-range forces.

(1-2-2) Constitution of Atom and Nucleus

The constitution of an atom from elementary particles is shown in Figure 1.2. The symbols "u" and "d" indicate quarks, shown in Table 1.1. We can see that protons, neutrons, and electrons are fundamental particles in the constitution of matter. Although there are numerous elementary particles, the only relevant particles in our earthly life and in nuclear reactors, which we are going to discuss, are photons and the particles that constitute material, that is, protons, neutrons, and electrons. Among these, the proton and neutron have approximately the same mass. However, the mass of the electron is only 0.05% that of these two particles. The proton has a positive charge and its absolute value is the same as the electric charge of one electron (the elementary electric charge). The proton and neutron are called nucleons and they constitute a nucleus. An atom is constituted of a nucleus and electrons that circle the nucleus due to Coulomb attraction.
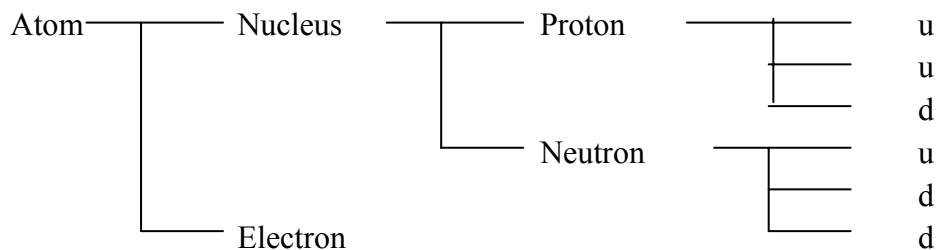
Figure 1.2   Constitution of an atom, No. 1

Species of atoms and nuclei are called elements and nuclides, respectively. An element is determined by its proton number (the number of protons). The proton number is generally called the atomic number and is denoted by Z. A nuclide is determined by both the proton number and the neutron number (the number of neutrons denoted by N). The sum of the proton number and neutron number, namely, the nucleon number, is called the mass number and is denoted by A (A=Z+N). Obviously, a nuclide can also be determined by the atomic number and mass number. In order to identify a nuclide, A and Z are usually added on the left side of the atomic symbol as superscript and subscript, respectively. For example, there are two representative nuclides for uranium, described as $^{235}_{92}U$ and $^{238}_{92}U$. If the atomic symbol is given, the atomic number can be

uniquely determined; thus Z is often omitted like ^{235}U and ^{238}U. The chemical properties of an atom are determined by the atomic number, so even if the mass numbers of nuclei are different, if the atomic numbers are the same, their chemical properties are the same. These nuclides are called isotopic elements or isotopes. If the mass numbers are the same and the atomic numbers are different, they are called isobars. If the neutron numbers are the same, they are called isotones. The above examples for uranium are isotopes. Summarizing these and rewriting the constitution of an atom, we obtain Figure 1.3.
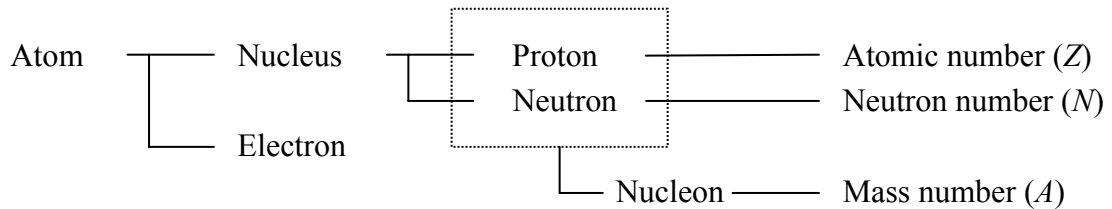

Figure 1.3   Constitution of an atom, No. 2

(1-2-3) Sizes of Atoms and Nuclei and Their Energy

The diameters of atoms and molecules are of the order of 10^{-10}–10^{-9} m. On the other hand, the diameters of nuclei are small, of the order of 10^{-15}–10^{-14} m. The size of molecules is often measured in Å (angstrom, 1 Å=10^{-10} m) and nm (1 nm=10^{-9} m). On the other hand, the size of nuclei is often measured in fm (femtometer, 1 fm=10^{-15} m). That is, the diameters of atoms and molecules are approximately 0.1–1 nm and the diameters of nuclei are approximately 1–10 fm.

Because of the uncertainty principle, a much higher energy is associated with a nucleus than with an atom or a molecule, as it is much smaller. Chemical reactions are measured in the unit of eV (where 1 eV is the energy acquired when a particle with one elementary electric charge is accelerated by a potential difference of 1 V in a vacuum). In contrast, the unit of MeV (1 MeV = 10^6 eV) is usually used for nuclear reactions.

An approximate, but rather more concrete explanation is given by the following. The n-th energy eigenvalue for a particle with mass m trapped inside a potential well of size L is given by the following equation.

$$E_n = N_n \frac{1}{2m} \left(\frac{\pi \hbar}{L} \right)^2$$

Here N_n is a constant determined by the quantum number n and $\hbar = 6.582 \times 10^{-16}$ eVsec is the value obtained by dividing Planck's constant by 2π. We let $n = 1$ and use the mass of a nucleon and the mass of an electron shown in Table 1.4 of Sec. (2-4). For an electron, $(1/2m)(\pi \hbar /L)^2$=3.8×10^{-15} eV if L=1 cm, giving a very small value. For an atom of size 0.1–1 nm, the energy is 38–0.38 eV. In the case of a proton, the energy is 200–2 MeV for a nucleus of size 1–10 fm.

(1-2-4) Mass of a Nucleus

The mass of a proton is approximately the same as that of a neutron, whereas the mass of an electron is much smaller than that of a proton or neutron. As a unit for measuring the mass of an atom (the atomic weight), the value obtained by dividing the mass of an atom with its mass number is convenient (this is called the 'atomic mass unit' with symbol 'amu' or 'u'). However, the sum of the masses of a proton and an electron is different from the mass of a neutron. In

addition, when nucleons are bound, the mass will generally decrease from the sum of the masses of the original nucleons (this will be explained later). Thus, it is necessary to use a specific standard nuclide to determine the atomic mass unit. Various nuclides have been proposed for this standard, but from 1962, international consensus has been to use the atomic weight of $^{12}_{6}\text{C}$ divided by 12 to obtain the standard 1 amu. The masses of the proton, neutron, and electron using this atomic mass unit are shown in Table 1.4. They are also shown in the unit of MeV/c^2, which will be explained later.

Table 1.4   Masses of proton, neutron, and electron.

Particle	amu	MeV/c^2
Proton	1.007276	938.280
Neutron	1.008665	939.573
Electron	0.000549	0.511

In a nucleus, nucleons are attracted to each other by the nuclear force. Nucleons in such a field try to take as low an energy state as possible. That is, when separate nucleons are combined together, the lowest energy state is taken and the excess energy is released. This energy is called the binding energy. The relationship between the energy E and mass M is the following, derived from Einstein's famous relativity theory:

$$E = Mc^2 .$$
(1-1)

Thus, the mass of the atom is smaller than the sum of the masses of nucleons and electrons that constitute the atom. This difference in mass is called the mass defect, $D(Z,N)$ for a nuclide with atomic number Z and neutron number N. For the mass of a hydrogen atom m_H and the mass of a neutron m_N, the mass of a neutral atom is expressed as follows:

$$M(Z,N) = Zm_H + Nm_N - D(Z,N) .$$
(1-2)

The binding energy can be expressed as follows using Eq. (1-1):

$$B(Z,N) = D(Z,N)c^2 .$$
(1-3)

The binding energy is equivalent to the mass defect, with the binding energy used when energy is being considered and the mass defect used when mass is being considered. The unit MeV is often used for the energy of nuclear reactions, with mass and energy converted according to the following relationship:

$$1 \text{ amu} = 931.5016 \text{ MeV/c}^2 ,$$
(1-4)

A term similar to the mass defect is the mass deviation (or mass excess), defined as the difference $M-A$, for M the mass in atomic mass units and A the mass number, which is an integer. It is important to clearly distinguish these terms.

Different nuclei have different mass defects. Accordingly, energy is absorbed or released

during a nuclear reaction. In addition, it is possible to determine the possibility of a certain reaction occurring by the size of the mass defect. Thus, it is very important to know the mass defect of a nuclide. In this section we are concerned with the state with the lowest internal energy of the nucleus. This state is called the ground state. States with higher internal energy are called excited states.

The most important force in the nucleus is the nuclear force. The nuclear force is a strong interaction, generated by the exchange of pions. The distance of interaction is very short, approximately 2 fm, and thus only neighboring nucleons interact with each other. Therefore, the contribution of the nuclear force to the mass defect is proportional to the mass number. For a_v, a suitable proportionality constant, the contribution is expressed as $a_v A$. If all the nucleons are surrounded by other nucleons, this expression is satisfactory. However, there are no nucleons outside the surface nucleons, and thus the binding energy is smaller to that extent. This is the so-called surface tension and is expressed as $-a_s A^{2/3}$. The second important force in a nucleus is the Coulomb force. Inside a nucleus, there are positive charges due to protons, but there are no negative charges. Therefore, a repulsive Coulomb force operates. This force exists among the protons. Its energy is obtained by dividing the product of the electric charges by the distance between them. In this case, the distance may be considered proportional to the size of the nucleus. If the volume of the nucleus is proportional to the mass number, the contribution of the Coulomb force to the mass defect is expressed as $-a_c Z^2 A^{-1/3}$. If these were the only forces existing among nucleons, a nucleus containing only neutrons would have strong binding because of the absence of the Coulomb force. However, this is not consistent with experimental results. In reality, in a strongly bound nucleus, the proton number and the neutron number are similar. Thus, there is symmetry between protons and neutrons, and the closer the proton and neutron numbers, the more stable the nucleus is. Thus, the expression $-a_I (N-Z)^2 A^{-1}$ is added to the mass defect. In addition to the above important terms, pairs of protons or of neutrons have a stabilizing property. Thus, when the proton number or the neutron number is even, the nucleus is more stable. This effect is expressed as $a_e \delta(Z,N) A^{-1/2}$, with the following function introduced:

$$\delta(Z,N) = \begin{cases} 1 : If\ both\ Z,N\ are\ even \\ \quad 0 : If\ A\ is\ odd \\ -1 : If\ both\ Z,N\ are\ odd \end{cases} \tag{1-5}$$

Weiszacker and Bethe have proposed the following emiempirical mass formula by adding these terms together:

$$B(Z,N) = a_v A - a_s A^{2/3} - a_c Z^2 A^{-1/3}$$
$$- a_I (N-Z)^2 A^{-1} + a_e \delta(Z,N) A^{-1/2} \ . \tag{1-6}$$

The terms on the right side are, from the left, the volume term, surface term, coulomb term, symmetry term, and even-odd term. The coefficients are determined so that the mass defect is consistent with the experimentally determined masses. An example set of coefficients determined by Wapstra in 1958 is shown below:

a_v=15.835 MeV
a_s=18.33 MeV
a_c=0.714 MeV
a_I=23.20 MeV

a_e=11.2 MeV .

This equation is simple, but it nicely reproduces the experimental data, with the errors for heavy nuclei less than 1%. However, for a detailed analysis of nuclear reactions, more accurate values are often necessary. In that case, please consult reference [1]. The binding energy per nucleon and contribution of each term will be shown later in Fig. 1.7.

In the derivation of the mass formula, we notice that for suitable values of A and N there may be a nuclide with the greatest binding energy per nucleon, that is, the most stable nuclide. In fact, ^{56}Fe has the largest binding energy per nucleon of 8.55 MeV. When A and Z depart from the suitable values, the binding energy decreases and the nuclide becomes unstable. When the binding energy is negative, the nucleus cannot exist. However, even when the binding energy is positive, not all nuclides can exist. There are numerous cases where a nuclide will decay to another nuclide with a larger binding energy. However, the number of such decays is limited and there are numerous nuclides in nature besides the most stable nuclides. This will be explained in a later section.

Nuclei also have a property that corresponds to the closed shells of electrons in an atom. Nuclei with a neutron number N or proton number Z of 2, 8, 20, 28, 50, 82, or 126 are especially stable compared with nuclei with numbers in the vicinity. These numbers are called magic numbers. They will be shown on the chart of nuclides in Fig. 1.6.

(1-2-5) Nuclear Reactions

In this section, nuclear reactions are briefly explained. A nuclear reaction is generally described as follows:

$$a + X \rightarrow Y + b \quad . \tag{1-7}$$

Here, a is an incident particle, X is a target nucleus, Y is a residual nucleus, and b is an emitted particle. Reactions where no a is involved are called decays.

Before and after the nuclear reaction, the total energy and momentum are conserved for the system. From these conservation laws, restrictions apply to particle energy and direction of motion in the reaction. In the laboratory coordinate system, the target nucleus X is considered to be at rest. Thus, the following equation holds based on the energy conservation law:

$$(M_a + M_X)c^2 + E_a = (M_b + M_Y)c^2 + E_b + E_Y \quad . \tag{1-8}$$

Here, relativity theory is ignored, and M_a, M_X, etc. represent the respective masses and E_a, E_b, etc. represent the respective kinetic energies in the laboratory coordinate system. We call the increase in kinetic energy due to the reaction the Q-value or the reaction energy:

$$Q = E_b + E_Y - E_a \quad . \tag{1-9}$$

It is clear that this also corresponds to the decrease in mass due to the reaction:

$$Q = \left[(M_a + M_X) - (M_b + M_Y)\right]c^2 \quad . \tag{1-10}$$

From this equation, the Q-value can be obtained from only the masses of the particles involved in the reaction (or from the mass defect, as described in the previous section). Thus, the Q-value does not depend on the energy of the incident particle.

The reaction equation is sometimes written by adding the *Q*-value to Eq. (1-7):

$$a + X \rightarrow Y + b + Q \quad .$$
(1-11)

The *Q*-value can take either a positive or negative value. When it is positive, the reaction is called an exoergic reaction. When it is negative, the reaction is called an endoergic reaction. An endoergic reaction cannot take place unless the energy of the incident particle *a* surpasses a certain minimum value. This minimum value is called the threshold energy and it can be obtained by the following equation:

$$E_{ath} = -Q \frac{M_a + M_X}{M_X} \quad .$$
(1-12)

When the residual nucleus *Y* is left in an excited state, the mass of *Y* is larger than the mass of the ground state M_Y. If we denote this mass by $M_Y '$, the *Q*-value for this reaction is expressed by the following equation, which is different from that for the ground state, as $Q'<Q$:

$$Q' = \left[(M_a + M_X) - (M_b + M_Y') \right] c^2 \quad .$$
(1-13)

In this case, the energy of the emitted particle E_b is clearly smaller. The residual nucleus *Y* in the excited state will eventually decay by some decay process.

In a nuclear reactor, reactions between neutrons and nuclei are important. However, I will explain this in detail later. In the next section, I will briefly explain the decay of nuclei and will then continue the explanation of the mass of a nucleus.

(1-2-6) Decay of a Nucleus

The decay of a nucleus is briefly explained in this section. Typical decays are α-decay, β-decay, and γ-decay, which emit α-rays, β-rays, and γ-rays, respectively. An α-ray is a nucleus of ^{4}He, a β-ray is an electron, and a γ-ray is a high-energy photon. In β-decay, a positron may be emitted, which is called β$^+$-decay. In order to distinguish the two cases, the ordinary decay in which an electron is emitted is sometimes called β$^-$-decay. As a competitive process for β$^+$-decay, orbital electron capture occurs when a nucleus takes in an orbital electron. As a competitive process for γ-decay, internal conversion occurs when an orbital electron is ejected, rather than a γ-ray being emitted. By α-decay, *Z* and *N* both decrease by 2. By β$^-$-decay, *Z* increases by 1 and *N* decreases by 1. By β$^+$ decay and orbital electron capture, *Z* decreases by 1 and *N* increases by 1. By γ-decay and the internal conversion, neither *Z* nor *N* change.

Some decays take place readily, while other decays rarely occur. The conservation laws for angular momentum, parity, etc. play a great role in this difference. However, I will omit a detailed explanation of this and will instead describe other important matters.

When a positively charged particle is emitted from a nucleus, the particle should normally have to overcome the potential of the Coulomb repulsive force, shown in Figure 1.4, since the nucleus also has a positive charge. In reality however, it is not necessary to overcome the potential peak, and a particle with an energy smaller than the peak energy can be emitted by the tunnel effect. However, the probability of this occurring rapidly decreases when the mass of the emitted particle becomes large or the height and thickness of the potential wall increase. Therefore, the emission of a heavy particle and reactions with low Q-value occur with difficulty. As a result, the α-particle is the only positively charged particle that is regularly emitted, and is generally emitted only from nuclei with large atomic numbers Z. However, α-particles can

occasionally be emitted from light nuclei, and a nucleus of proton or carbon may occasionally be emitted.
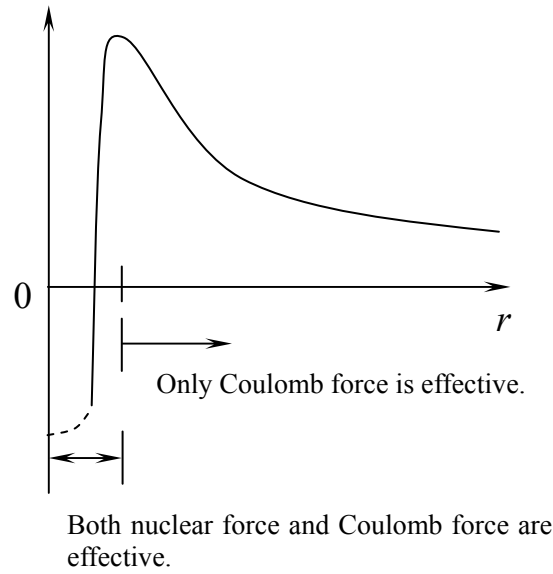

Figure 1.4   Potential of the Coulomb repulsive force in nuclear decay.

In γ-decay, there is no Coulomb barrier since the emitted particle is a photon. In internal conversion, which competes with γ-decay, there is no barrier since the emitted particle is an electron, which is attracted by the nucleus. In β-decay, there is no barrier for neutrinos, since the interaction of a neutrino with other material can be ignored. When the other emitted particle is an electron, it is attracted by the nucleus, and thus there is also no barrier. In the case of a positron, there is a Coulomb barrier. Nevertheless, the mass of a positron is smaller than that of an α-particle, and thus it can easily pass through the barrier. However, in nuclides with large atomic numbers, $β^+$-decay with low decay energy rarely takes place since orbital electron capture, which is a competitive process, dominates. Since β-decay is a weak interaction and γ-decay is an electromagnetic interaction, γ-decay takes place more easily than β-decay. Spontaneous fission is another important decay for heavy nuclei. In this case, a Coulomb repulsive force even stronger than for α-decay applies, and the masses of the emitted particles are large, therefore the parent nucleus must have a sufficiently high energy. Since the neutron has no Coulomb barrier, a neutron can easily jump out of a nucleus if energy permits. Although it is not appropriate to call this a decay, it is important in relation to the later-described delayed neutron, which accompanies nuclear fission.

The rate of decay is naturally proportional to the number of nuclides N under consideration and is expressed by the following equation:

$$\frac{dN}{dT} = -\lambda N \quad .$$
(1-14)

Here, the proportionality constant λ is unique to the particular nuclide and is called the decay constant. If we let the number of nuclides at $t=0$ be N_0, the following solution is obtained for Eq. (1-14):

$$N = N_0 \exp(-\lambda t) \quad .$$
(1-15)

The time necessary for N to become half of N_0 is called the half life. From Eq. (1-15), the half life $T_{1/2}$ can be expressed using λ in the following way:

$$T_{1/2} = \frac{\log 2}{\lambda} = \frac{0.69315}{\lambda} \; . \tag{1-16}$$

The mean life of a nucleus τ is expressed by the following equation:

$$\tau \;=\; \frac{1}{N_0} \int_0^\infty t\,\lambda\,N dt \;\;=\; \frac{1}{\lambda} \; . \tag{1-17}$$

The capability to emit radiation is called radioactivity. Radioactive strength is expressed by the unit becquerel (Bq), an SI unit. One decay per second is 1 Bq. However, the traditionally used unit, the curie (Ci), is still frequently used. The two units are converted according to the following:

$$1\,\mathrm{Ci} \;=\; 3.7 \times 10^{10}\,\mathrm{Bq} \; . \tag{1-18}$$

(1-2-7) Distribution of Nuclides and Nuclear Fission/Nuclear Fusion

In the previous section, it is explained that three kinds of decays can easily take place. The decays are α-decay, β-decay, and γ-decay, but their order of likelihood is γ-decay, β-decay, α-decay. In γ-decay, the nucleus does not change.
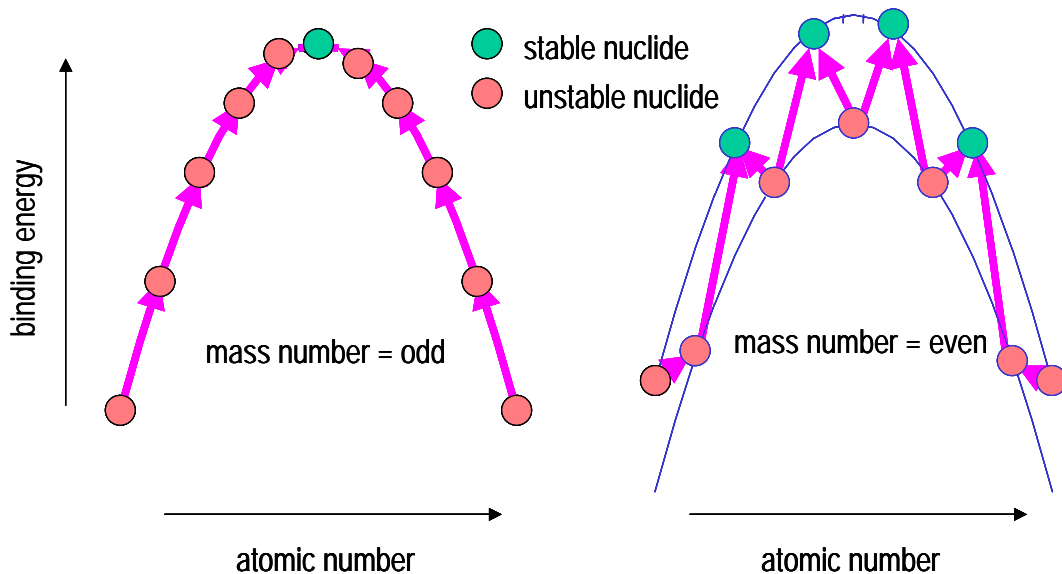
Figure 1.5   Binding energy change in β-decay and the direction of the decay.

In β-decay, the next most likely decay, the mass number A does not change, but the atomic number Z changes. Plotting neutron number N against atomic number Z following β-decay gives a slope of 45°. On this line, the binding energy (mass defect) changes as shown in Figure 1.5 (See Eq. (1-6)). When A is odd, the last term of Eq. (1-6) becomes zero and the points representing the

binding energy for the respective nuclei stay on a parabolic curve. The nuclide at the highest point is a stable nuclide and is generally uniquely determined; nuclides with a higher Z than this decay by β^+-decay and nuclides with the lower Z decay by β^--decay. When A is even, the last term of Eq. (1-6) is positive if Z is even and odd if Z is negative. Therefore, the points representing the binding energy of respective nuclei are alternately on either of two parabolic curves. Thus, there is a possibility that multiple stable nuclides exist, and these stable nuclides are alternately located between unstable nuclides. Nuclides may also undergo a change in A, which is likely to take place through α-decay; however, A should be very large in this case. As a result of these decays, the only naturally-occurring nuclides are those shown in Figure 1.6.
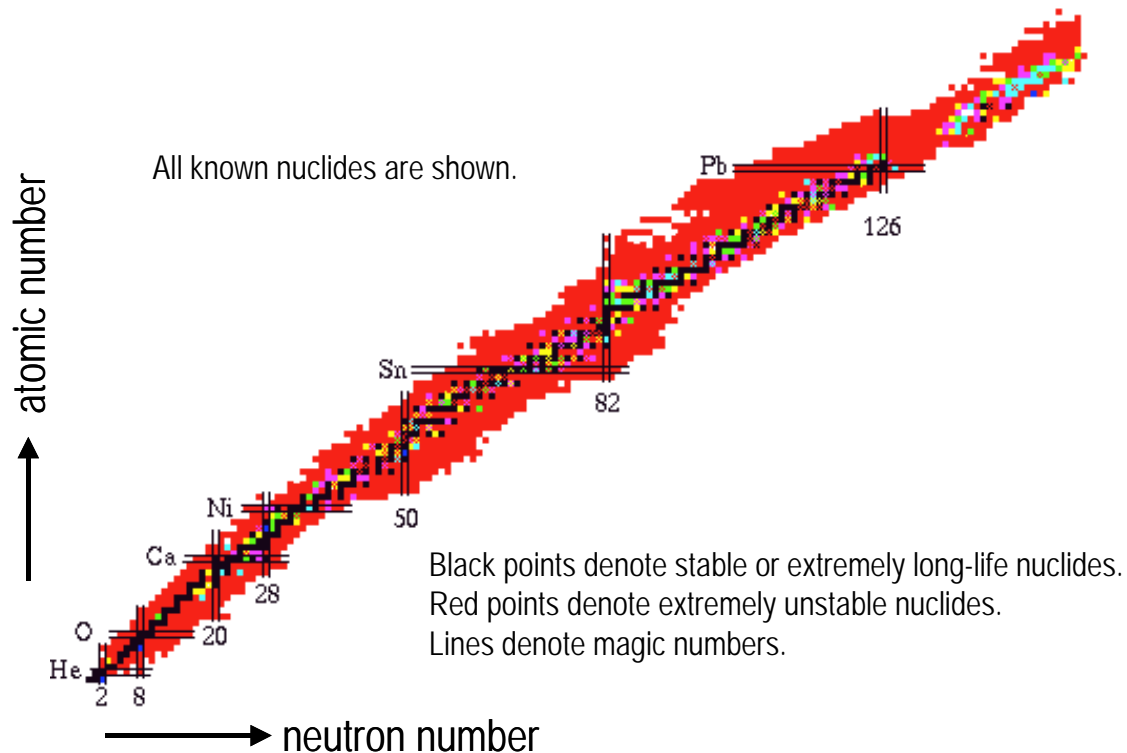
Figure 1.6   Chart of the nuclides[2].

In Figure 1.6, we can see that the curve along the stable nuclides is convex, curving downward at high A, because of the balance of the coulomb and symmetry terms. Therefore, when a heavy nuclide fissions into two nuclides of approximately equal mass, the resulting nuclides are unstable, having too many neutrons. In reality, two or three neutrons are emitted during fission and most fission products will decay by β-decay.

If the mass number A of naturally-occurring nuclides is plotted as the abscissa and the binding energy is plotted as the ordinate, Figure 1.7 is obtained. Where A is small, the surface term is large, and where A is large, the coulomb term is large. According to this figure, we can see that a nuclide with small A can fuse to a nuclide with a large binding energy and release energy. Similarly, a nuclide with large A can fission into nuclides with large binding energies, releasing energy. By nuclear fission, two fission products of approximately equal mass are generated.

Figure 1.7   Binding energy per nucleon and contribution of each term.[2]

(1-3) Neutron Nuclear Reactions

(1-3-1) Neutron Reactions and Characteristics

Compared with chemical reactions, nuclear reactions are much less likely to occur. The first reason for this is, as described in Sec. (2-1), that a nucleus is much smaller than an atom and molecule, and collisions are less likely to tak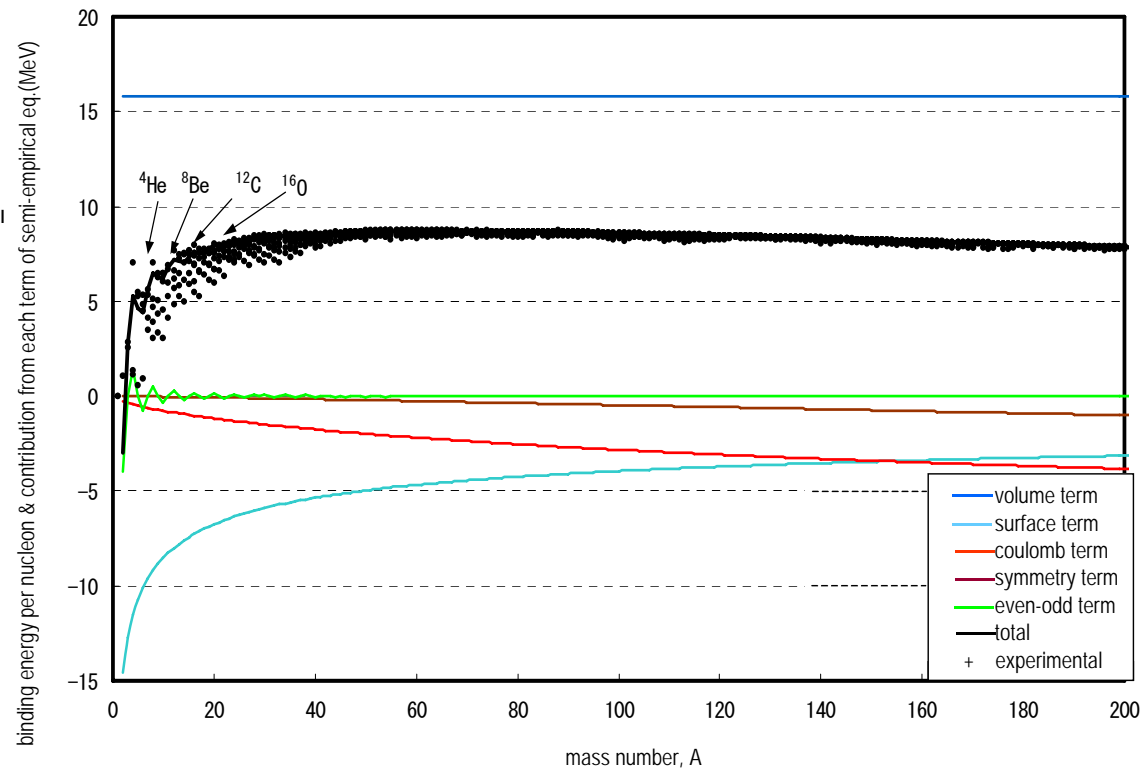e place. The second reason is that nuclei are positively charged, and thus have difficulty in approaching each other because of the repulsive Coulomb force. High energy is usually required to overcome the Coulomb force. Since the neutron has no electric charge, there is no Coulomb barrier and a high energy is not necessary. Moreover, when the energy is low, quantum mechanics dictates that the wavelength increases, and thus reactions can often take place more easily. According to de Broglie, a neutron with momentum p has the following wavelength:

$$\lambda = h \big/ p \quad . \tag{1-19}$$

where, h is Planck's constant. If we use energy instead of momentum, we obtain the following:

$$\lambda = 2.86 \times 10^{-11} E^{-1/2} \quad (m) . \tag{1-20}$$

Here, eV is used as the unit of E. This energy is extremely large compared with that of a nucleus, as described in Sec. (2-1). For a neutron velocity v, the neutron will behave as if the size of the neutron is proportional to $1/v$.

There are various neutron reactions, as shown in Figure 1.8. The important reactions are explained in detail below. In this figure, nuclear fission is classified as absorption even though neutrons are emitted.
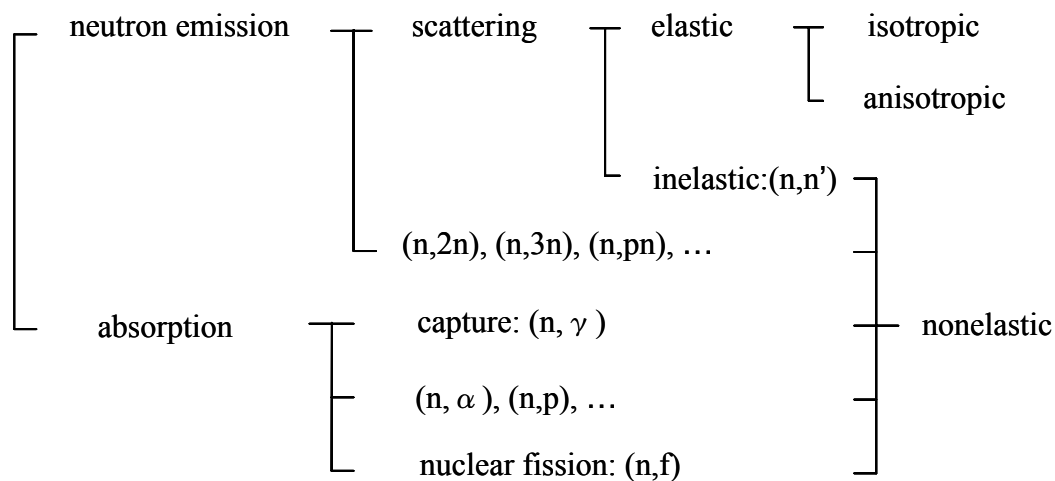

Figure 1.8   Neutron reactions.

Although a neutron inside a stable nucleus is stable, an isolated neutron changes to a proton by β-decay. The half life of an isolated neutron is short, only 10.37 minutes, however, this is long when we consider the behavior of neutrons inside a nuclear reactor. We need not consider the

decay of neutron during neutron transport in a nuclear reactor.

The types and rates of neutron reactions depend upon the nucleus under collision and the neutron energy. Most reactions other than elastic scattering become threshold reactions, mentioned in Sec. (2-5), for many nucleus. They occur when the neutron energy is more than about 1 MeV. The elastic scattering is isotropic for low energy scattering, but becomes anisotropic for higher energy. For higher energy most reactions show complicated behavior. Heavier nuclides also show complicated behavior.

(1-3-2) Scattering of Neutrons

Scattering is a reaction in which the emitted particle is of the same kind as the incident particle. There are two kinds of scattering, elastic scattering and inelastic scattering. Sometimes any reaction other than elastic scattering is called nonelastic scattering. In the analysis of neutron distributions, the neutron emission reaction is important and neutron emission reactions other than elastic scattering are often considered together.

I will start with an explanation of elastic scattering. This reaction can be handled in the same way as elastic collisions in classical mechanics, since the kinetic energy and momentum are conserved. The mass of a nucleus in the units of neutron mass is expressed as A. (This number is close to the mass number, and therefore the same symbol is used as the mass number. Please do not be confused.) If we let the neutron energies before and after the collision be E and E', the following equation can be obtained:

$$\frac{E'}{E} = \frac{1}{2}\left[(1 + \alpha) + (1 - \alpha)\mu_C\right] \quad . \tag{1-21}$$

The following will hold:

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 \tag{1-22}$$

$$\mu_C = \cos\theta_C \quad . \tag{1-23}$$

θ_C is the scattering angle in the center-of-mass coordinate system. From Eq. (1-21), the following range of energy change is obtained by scattering for a neutron with an initial energy E:

$$E \geqq E' \geqq \alpha E \quad . \tag{1-24}$$

Here, α is the maximum rate of energy loss due to the collision with a nucleus of mass A. The lighter the nucleus, the larger the energy loss by the neutron.

When the energy of a neutron is low (usually less than 100 keV), only elastic scattering due to S waves takes place, which is isotropic in the center-of-mass coordinate system. If we denote the probability of scattering by $d\mu_c$ as $P(\mu_C)d\mu_C$, then we have the following:

$$P(\mu_C) = \frac{1}{2} \quad . \tag{1-25}$$

Thus, if we represent the probability for a neutron with energy E taking an energy E' after scattering with a small range dE' as $P(E \rightarrow E')dE'$, we have the following:

$$P(E \rightarrow E') = P(\mu_C)\frac{d\mu_C}{dE'} = \frac{1}{(1-\alpha)E} \quad . \tag{1-26}$$

The average value of ln (E/E'), which is the logarithmic value of the rate of energy change for a neutron with energy E, is denoted by ξ and is called the logarithmic energy decrement. From Eq. (1-26) we obtain the following:

$$\xi = 1 + \frac{\alpha}{1-\alpha}\ln \alpha \quad . \tag{1-27}$$

The average value of the cosines of the scattering angles in the laboratory coordinate system $\overline{\mu}_L$ can be obtained in the following way:

$$\overline{\mu}_L = \frac{2}{3A} \quad . \tag{1-28}$$

From this equation, it can be seen that for heavier nuclei, the scattering becomes isotropic in the laboratory coordinate system. The values α, $\overline{\mu}_L$, and ξ for some nuclei are shown in Table 1.5.

Table 1.5   Moderation characteristics for representative nuclides by elastic scattering.

Material	A	α	$\overline{\mu}_L$	ξ
Hydrogen	1	0	0.667	1.000
Deuterium	2	0.111	0.333	0.725
Helium	4	0.225	0.168	0.425
Beryllium	9	0.640	0.074	0.206
Carbon	12	0.716	0.056	0.158
Uranium	238	0.983	0	0.0084

In the case of inelastic scattering, a nucleus under collision is excited and the energy of the scattered neutron decreases by the amount of the excitation energy. In order for excitation to occur, it is necessary that there be a nuclear energy level above the initial energy level by an amount of energy equal to the excitation energy. Generally, the heavier the nuclide, the more densely the levels are distributed, and thus heavier nuclides have a larger cross-section for inelastic scattering.

(1-3-3) Nuclear Fission

As described in Sec. (2-4), the main forces operating inside a nucleus are due to the volume term and surface term. This causes the nucleus to behave like a liquid drop. Therefore, if energy is applied from the outside, oscillation modes are excited in the same way as for a liquid drop. In this way, a nucleus can fission into two pieces, which is the process known as nuclear fission.

This type of nuclear fission is observed in heavy nuclei. Among the naturally-occurring nuclides, only ^{235}U can fission by thermal neutrons. If the energy of the neutrons is increased, ^{238}U and ^{232}Th can fission. Nuclear fission by a thermal neutron is called thermal fission and that by a fast neutron is called fast fission. Thermally fissionable material is called fissile material,

and includes ^{233}U, ^{239}Pu, and ^{241}Pu in addition to ^{235}U. The nuclide ^{233}U can be prepared from ^{232}Th, and ^{239}Pu, and ^{241}Pu can be prepared from ^{238}U by neutron absorption. Material that can produce fissile material is called fertile material. The nuclide ^{252}Cf can fission without being irradiated by neutrons, a type of nuclear fission called spontaneous fission.

The only naturally-occurring elements that are useful as nuclear fuel are uranium and thorium. Uranium of natural composition is called natural uranium. Natural uranium contains 0.0054% ^{234}U, 0.720% ^{235}U, and 99.275% ^{238}U. Natural thorium contains 100% ^{232}Th.

When nuclear fission takes place, the nucleus splits into two fission fragments of approximately equal mass. Fission fragments are usually called fission products. The distribution of those mass numbers is shown in Fig. 1.9, showing results of thermal fission, for which case the distribution is asymmetrical. This asymmetrical distribution can be attributed to the stability of magic numbers, which were described in Sec. (2-2). In the case of fast fission, this asymmetrical distribution is not prominent. In this figure, the total yield per fission is 200%, since two fission products usually appear per one fission.
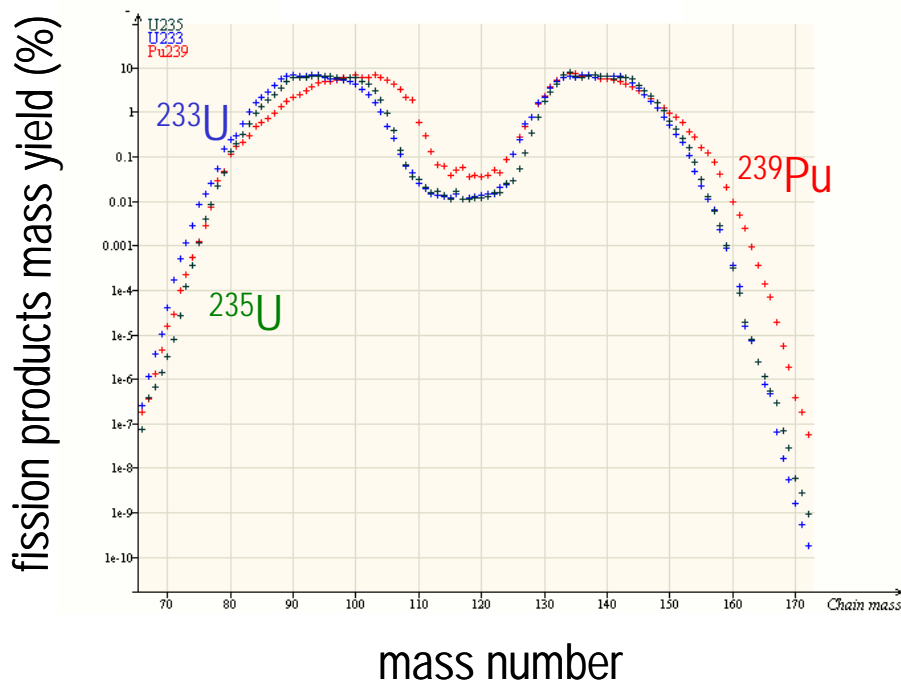
Figure 1.9 Fission product mass yield per fission induced by thermal neutrons for important fissile nuclides[2]. Total yield is 200%.

As seen in Fig. 1.7, approximately 1 MeV/nucleon of mass excess is reduced by nuclear fission. This corresponds to about 200 MeV for the total number of nucleons, which is the energy generated by nuclear fission.

If we assume that a nucleus splits into fission products of approximately equal mass by nuclear fission, the fission products would have too many neutrons compared with stable nuclei, as we can see from Fig. 1.6. Therefore, neutrons are usually generated at the time of nuclear fission. The number of generated neutrons increases as the energy of the colliding neutron increases or the mass number of the nucleus increases. When a thermal neutron is incident on ^{235}U, about 2.5 neutrons are generated. This enables a chain reaction, which I will describe next, and indicates that nuclear fission can be effective in generating energy. The energy of these neutrons is distributed as if the neutrons were in thermal motion in the nucleus. The distribution

for ^{235}U is given by the following equation:

$$x(E) = 0.453 \exp(-1.036E) \sinh(2.29E)^{0.5} \quad .$$ (1-29)

Here, the unit of the neutron energy E is MeV. Fig. 1.10 shows the plotted distribution. Among fission products, there are numerous nuclides that still have too many neutrons even after neutron-generating nuclear fission. These nuclides generally decay by β-decay, changing into stable nuclides. However, some nuclides decay by emitting neutrons. In order to distinguish them, the neutrons emitted at the time of nuclear fission are called prompt neutrons, while the neutrons emitted later are called delayed neutrons. Delayed neutrons play an important role in the operation of nuclear reactors.
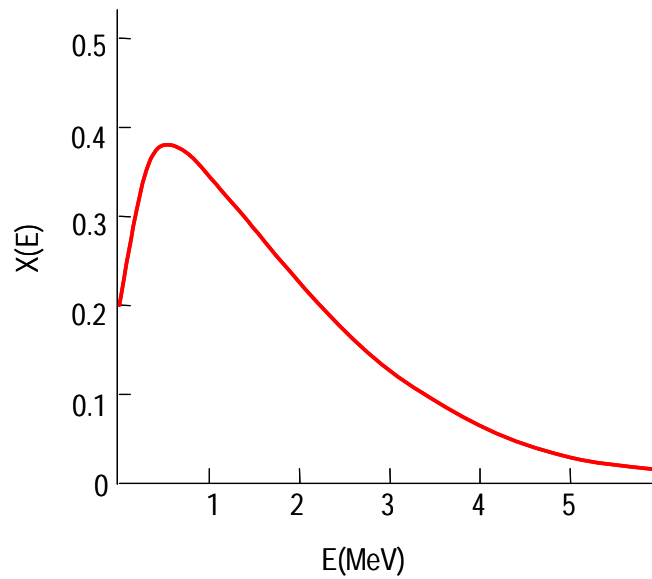
Figure 1.10   Fission neutron energy spectrum.

(1-3-4) Chain Reaction

Based on Fig. 1.8, neutrons behave in a nuclear reactor as shown in Fig. 1.11. If the number of neutrons satisfies the following equation, the number of neutrons will never change:

neutrons generated by nuclear fission + neutrons increased by (n,2n), etc.
= absorbed neutrons + leaked neutrons   . (1-30)

This is called the critical state. However, the phenomenon is stochastic and the actual number constantly fluctuates. If the right side of Eq. (1-30) is larger than the left side, the number of neutrons will increase, which is called the supercritical state. If the right side of the equation is smaller than the left side, the number of neutrons will decrease, which is called the subcritical state.

In succeeding generations of a chain reaction, the ratio of the number of neutrons in one generation to the number of neutrons in the preceding generation is called the neutron multiplication factor or simply multiplication factor. The multiplication factor is usually denoted

by *k*. It is expressed as follows:

$$k = \frac{\text{Number of neutrons in one generation}}{\text{Number of neutrons in the preceding generation}} \quad . \tag{1-31}$$
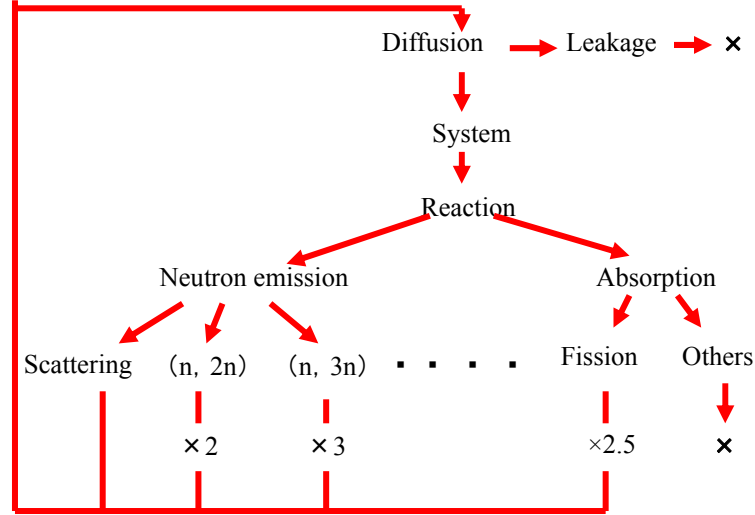
Figure 1.11   Neutron evolution in a nuclear reactor.

When a nuclear reactor can be assumed to be infinitely large and the neutron leakage is zero, the multiplication factor is called the infinite medium neutron multiplication factor or simply infinite multiplication factor, and designated by k_∞. It is convenient to use k_∞ to express the characteristics of a material. When the size of a nuclear reactor is taken into account and the neutron leakage is correctly handled, the multiplication factor is called the effective neutron multiplication factor and designated by k_{eff}. A critical state is easily expressed by k_{eff}, that is, when $k_{eff}=1$, the state is critical, when $k_{eff}<1$, it is subcritical, and when $k_{eff}>1$, it is supercritical.

(1-3-5) Neutron Flux and Cross-section

When we consider a reaction of a neutron and a nucleus, the probability that the reaction takes place is considered to be proportional to the size of the nucleus and the distance that the neutron travels per unit time.   Thus, to express the quantity of neutrons, it is more convenient, as shown below, to use the product of the neutron number density *n* and the velocity *v* rather than to use the neutron number density:

$$\phi(r, E, t) = vn(r, E, t) \quad . \tag{1-32}$$

This quantity is called the neutron flux. When the neutron flux is considered with respect to the energy, it is often called the neutron spectrum. The reaction rate *R* can be expressed using the neutron flux as shown below:

$$R(r,t) = \int_0^\infty N\sigma(E)\phi(r,E,t)dE \quad .$$

<div align="right">(1-33)</div>

Here, N is the density of the target nucleus and σ is a proportionality constant. Since σ is considered the cross-section of the target nucleus that a neutron sees, it is called the cross-section. Note that the cross-section is dependent on the neutron energy because the size of the reaction is dependent on the energy as described above. Since σ is per nucleus, it is often more specifically called the microscopic cross-section. The microscopic cross-section is a very small value and it is normally measured in the units of 1 barn=10^{-28} m^2. Usually, σ appears as a product with N as shown below:

$$\Sigma = \sigma N \quad .$$

<div align="right">(1-34)</div>

Σ is called the macroscopic cross section. The dimension of the macroscopic cross-section is m^{-1} since the dimensions of N are m^{-3}; it does not have the dimensions of area.

The cross-section is defined for each reaction. The sum of the cross-sections for all reactions is called the total cross-section. This corresponds to the probability of collision.

(1-4) Nuclear Reactors and their Structures

(1-4-1) Thermal Reactor

As mentioned in Sec. (3-1), for various neutron energies, reactions of different kinds and different sizes take place. If the energy of a neutron is lowered, its wavelike behavior and the reaction cross-section will increase. The amount of this increase depends upon the nuclide and reaction. The reaction cross-section of a thermal neutron depends significantly upon the target nuclide. The cross-section of ^{235}U nuclear fission is shown in Figure 1.12. The nuclear fissions of ^{233}U, ^{239}Pu, and ^{241}Pu by thermal neutrons also have very large cross-sections. If the energy of a neutron is lowered to a thermal level, the achievement of criticality becomes easy. This is because as the neutron energy is decreased the cross-section for fission increases faster than the absorption cross-section of material in the reactor other than the fuel. A nuclear reactor with a large fission rate by thermal neutrons is called a thermal reactor.
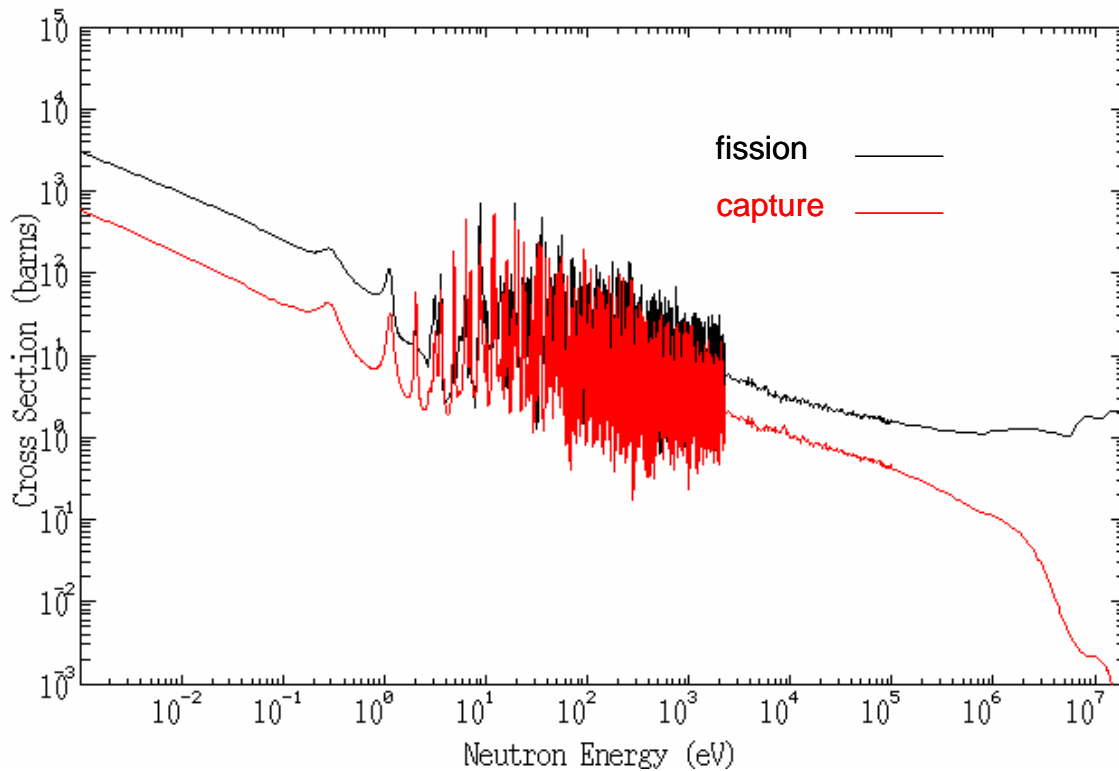
Figure 1.12   Fission and capture cross sections for ^{235}U[2]

As shown in Fig. 1.10, neutrons generated in nuclear fission have very high energy, and thus it is necessary to lower the energy in a thermal reactor. In order to moderate neutrons, the scattering explained in Sec. (3-2) can be used. In the high energy region, inelastic scattering and the (n, 2n) reaction can be used effectively. When the energy is lowered, however, these cross-sections are lost. Therefore, elastic scattering is the only useful moderation method over the wide energy region required to produce thermal neutrons. The rate of energy loss by elastic scattering is expressed by ξ in Eq. (1-27). Light nuclides have higher values, as shown in Table

1.6. Thus, neutrons generated in fission collide with light nuclei and are moderated to thermal neutrons. Material used to moderate neutrons is called a moderator. A moderator should be a light nucleus, but at the same time, it should have a small neutron capture cross-section. In order to express the performance of the moderator the following are used:

$$\text{moderating power} = \xi\Sigma_S \qquad\qquad\qquad (1\text{-}35)$$

$$\text{moderating ratio} = \xi\Sigma_S/\Sigma_a \quad . \qquad\qquad\qquad (1\text{-}36)$$

Values of these for typical moderators are shown in Table 1.6. For reference, the values for ^{238}U are also shown. (^{238}U is not a moderator, but is shown for comparison.) We can easily recognize differences due to the different mass numbers.

Table 1.6   Characteristics of typical moderators.

Moderator	A	α	ξ	Density (g/cm^3)	# of collisions From 2MeV To 1eV	$\xi\Sigma s$ [cm^{-1}]	$\xi\Sigma s/\Sigma a$
H	1	0	1	gas	14	—	—
D	2	.111	.725	gas	20	—	—
H$_2$O	—	—	.920	1.0	16	1.35	71
D$_2$O	—	—	.509	1.1	29	0.176	5670
He	4	.360	.425	gas	43	1.6×10^{-5}	83
Be	9	.640	.209	1.85	69	0.158	143
C	12	.716	.158	1.60	91	0.060	192
^{238}U	238	.983	.008	19.1	1730	0.003	.0092

As explained in Sec. (3-3), natural uranium contains only a small amount of fissile ^{235}U, with the rest being mostly ^{238}U. As shown in Fig. 1.13, ^{238}U shows a very large absorption for neutrons at an energy of 6.67 eV. This type of absorption is called resonance absorption. We can see that there are also many resonance absorptions for energies higher than this. Therefore, if natural uranium is used as a fuel, many neutrons are absorbed by ^{238}U and it is difficult to make the nuclear reactor critical. The most direct method to solve this problem is to enrich ^{235}U. However, enrichment is very costly. Another good method is to allow suitable separation of fuel and moderator in the reactor.

The separation of fuel and moderator is called a heterogeneous arrangement. Inside the moderator, both diffusion and moderation of neutrons take place. Since the nucleus of the fuel is heavy, it barely moderates neutrons, and thus, inside the fuel, diffusion is the dominant neutron motion. If the reactor is heterogeneous, neutrons scattered in the fuel tend to have successive collisions inside the fuel, and neutrons scattered in the moderator tend to have successive collisions inside the moderator. Thus, neutrons generated by nuclear fission in the fuel are not moderated inside the fuel, instead they enter the moderator region and gradually lose their energy there by moderation. When a certain low energy is reached, most neutrons diffuse from the moderator region. In the energy region with large resonance absorption, neutrons diffusing from the moderator region to the fuel region are mostly absorbed on the surface of the fuel region, and thus they cannot enter the interior of the fuel region. This effect is called self-shielding. Most neutrons are finally moderated to thermal neutrons in the moderator region and enter the fuel

region after repeated diffusion. They are then absorbed by ^{235}U. If the ratio between the fuel surface area and the volume is reduced by making broad fuel rods, self-shielding can greatly reduce resonance absorption. In light-water reactors, which are currently the most commonly operated reactors, neutron absorption by protons is considerable, enriched uranium is used and a heterogeneous arrangement is adopted.
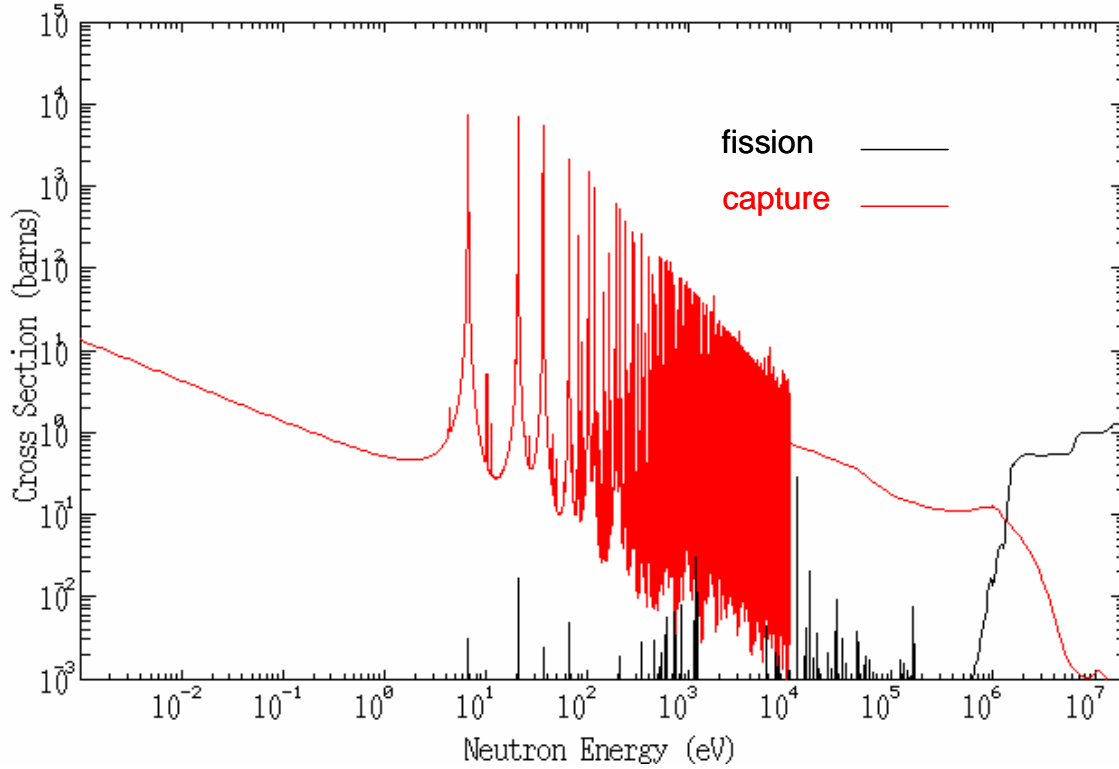
Figure 1.13   Cross sections for ^{238}U. [2]

(1-4-2) Breeder Reactors

Thermal reactors have the following problems. When the neutron energy becomes large, the fission cross-section increases and the capture cross-section also increases at almost the same rate. The number of neutrons emitted when one neutron is absorbed in the nucleus expressed as η is:

$$\eta = v \frac{\sigma_f}{\sigma_f + \sigma_c} \qquad . \tag{1-37}$$

Here, σ_f and σ_c are the cross-sections for fission and capture, respectively, and v is the average number of emitted neutrons per nuclear fission. The value η depends on the energy of the colliding neutrons, as shown in Fig. 1.14. For thermal neutrons, η is about 2, however, when the energy is more than 0.1 MeV, η increases rapidly. If many neutrons are generated in this way, not only can a chain reaction be maintained, but it may also be possible that there will be excess neutrons. If we let ^{238}U absorb these neutrons, ^{239}Pu can be produced, as mentioned before. That is, we can produce fissile material at the same time as we consume fissile material. The number

of newly generated fissile atoms per consumed fissile atom is called the conversion ratio. If the value η is sufficiently larger than 2, it is possible to obtain a conversion ratio larger than 1. Thus, it is possible to generate more fissile material than is consumed. This is called breeding, and the conversion ratio in this case is often called the breeding ratio and this type of reactor is called a breeder reactor. In other words fissile material can be bred using fast neutrons in a fast breeder reactor.
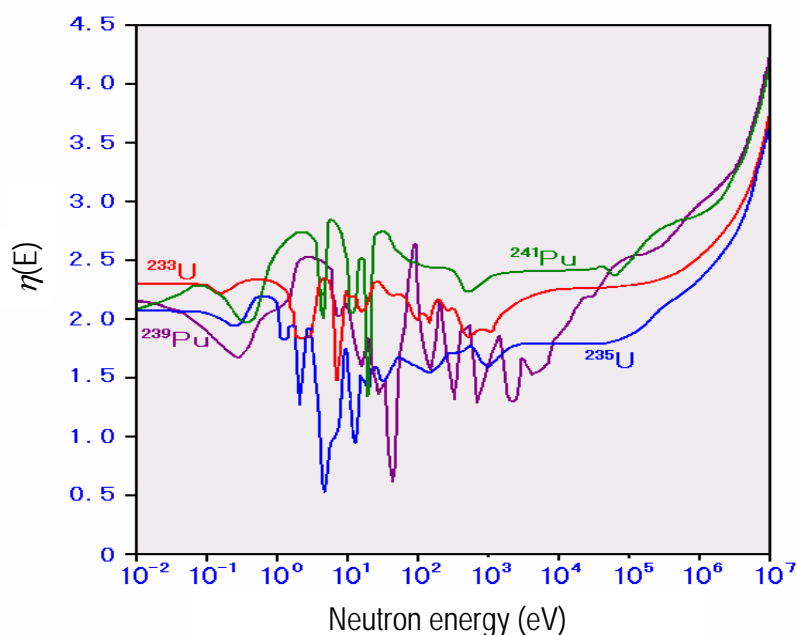

Figure 1.14 η-values for important fissile nuclides. [2]

Looking carefully at Figure 1.14, we can see that η for ^{233}U is larger than 2 in the region of thermal neutrons. Thus, it seems possible to perform breeding with thermal neutrons also. The nuclide ^{233}U can be prepared from ^{232}Th. However, since the margin of the neutron excess is very small in this case, ingenuity is required. A breeder reactor using thermal neutrons is called a thermal breeder reactor.

(1-4-3) Components of Nuclear Reactors

A thermal reactor consists of a fuel element, moderator, reflector, shielding, neutron absorber, coolant, and structural material. In the fuel element, nuclear fuel is generally covered by cladding. The fuel element is located in the core of the reactor. The moderator has already been explained in Sec. (4-1). The reflector is placed around the core to reflect leaked neutrons back to the core. For the reflector, the same material as that of the moderator is generally used. The shielding is placed outside the reflector so that radiation does not leak from the reactor, and the outside is shielded against neutrons and γ-rays.

The neutron absorber is used at the start-up and shut-down of the reactor and also to control the power output. The neutron absorber is called control material and is generally used in the form of a control rod. With the progress of burnup, the fissile material in the fuel decreases and fission products accumulate, which decreases the effective neutron multiplication factor. When continuous operation is necessary, the fuel is usually loaded so that k_{eff}>1 and then adjusted to

k_{eff}=1 by inserting the neutron absorber. When the amount of fissile material has decreased and fission products have accumulated with the progress of burnup, some of the neutron absorber can be removed. Thus, the neutron absorber is also used to maintain the reactor in a critical state over a long term. This will be explained again later.

The coolant conveys the energy generated in the reactor, in the form of heat, to the outside. These reactor components can all be separate parts, or some of them may play several roles. For example, the light water (in order to distinguish normal water from heavy water, it is called light water) used in light-water reactors acts as moderator, reflector, and coolant. Cooling of the reactor is important for safety, and is also very important in extracting the energy from the reactor, as is done in all types of power reactors presently operated. Therefore, thermal analysis of nuclear reactors is a very important field and will be covered in detail in another course.

In a fast reactor, neutrons are used without moderation. The components of a fast reactor are the same as for a thermal reactor, except for the moderator. However, a region called the blanket is normally placed between the core and reflector. Natural uranium or depleted uranium from enrichment or a reprocessing plant is loaded into the blanket,. The purpose of this is to prepare fissile plutonium by allowing ^{238}U to absorb neutrons that have leaked from the core.

Water reactors, high-temperature gas-cooled reactors, and fast reactors are presently used for power generation or propulsion or are close to being in actual use. An overview of these reactors is given in Table 1.7.

Table 1.7   Typical Nuclear Reactors

	Moderator	Coolant	Neutrons	Breeding	Purpose	Status
Water reactor	water	water	thermal	no	power	practical use
HTGR*	graphite	He	thermal	no	multi-purpose	development
Fast reactor	none	Na	fast	yes	power	development

*High Temperature Gas Cooled Reactor

Water reactors can be either light-water reactors or heavy-water reactors. The light-water reactor is the predominant power reactor. Light-water reactors include boiling-water reactors (BWR, Figure 1.15), in which the coolant is boiled in the core, and pressurized-water reactors (PWR, Figure 1.16), in which boiling is suppressed under high pressure. In a boiling-water reactor, power is generated by directly sending steam to a turbine. In a pressurized-water reactor, secondary cooling water is evaporated in a steam generator and the generated steam is sent to the turbine. Since the core in a heavy-water reactor is large, the moderator and coolant are generally segregated. The moderator is placed in an atmospheric vessel and the coolant is placed in a pressure tube. Either light water or heavy water is used as coolant. Usually, light water is used in the boiling-water type and heavy water is used in the pressurized-water type.
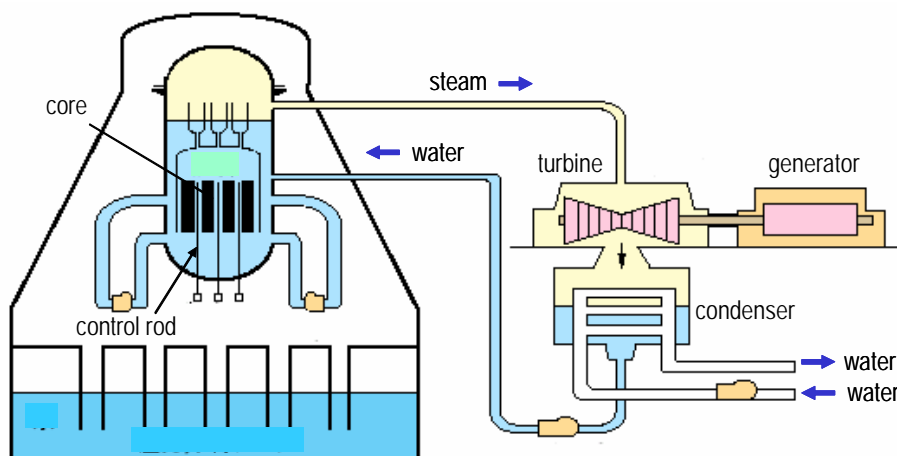
Figure 1.17   Boiling-water reactor (BWR).
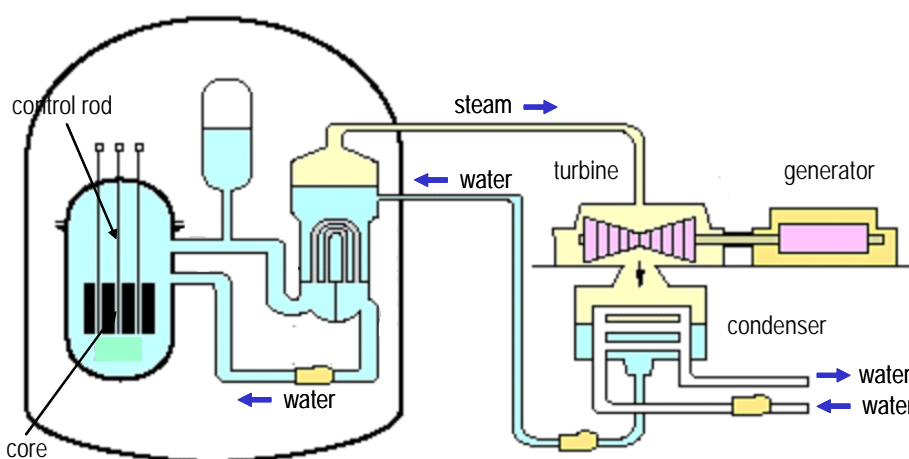
Figure 1.18   Pressurized-water reactor (PWR).

Currently under aggressive development is the high-temperature gas-cooled reactor, in which graphite is used as a moderator. Helium is used as coolant and higher temperatures can be obtained than are possible in other reactors. The high-temperature gas-cooled reactor is categorized into two types by the use of different fuel: the block-fuel type and pebble-bed type. Fig. 1.20 shows the pebble-bed reactor, developed as small modular reactors. Other reactors in which graphite is used as the moderator are the Calder Hall reactor, in which carbon dioxide is used as coolant, and the RBMK reactor, in which water is used as coolant. However, these reactors are gradually disappearing.
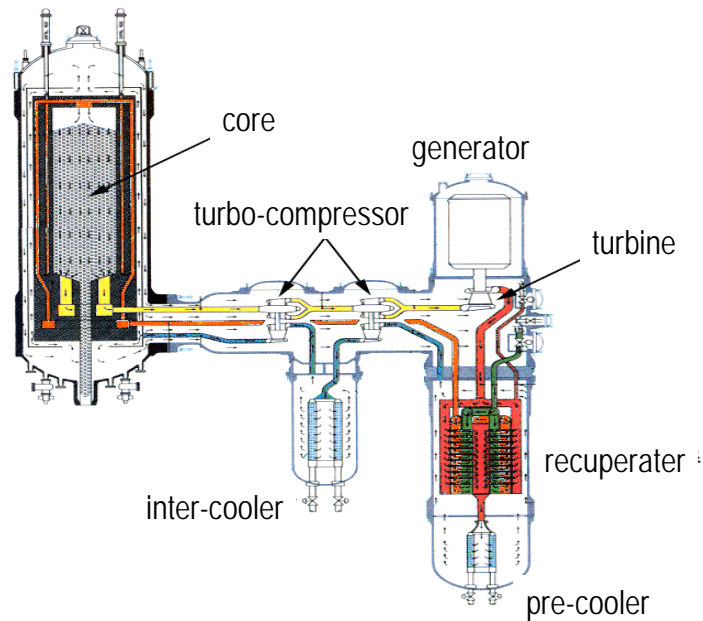
Figure 1.19   High-temperature gas-cooled reactor.

In most fast reactors (Fig. 1.20), a liquid metal, sodium, is used as coolant so that neutrons are not moderated. In these reactors, steam is also eventually generated. Since the contact of radioactive sodium and water is dangerous, a secondary sodium loop is installed between the primary sodium loop and the water. To avoid sodium-water reaction, lead or lead-bismuth is being experimented with as coolant. Another design uses gas such as helium or carbon dioxide as coolant since the density of gas is small and hardly reacts with neutrons.
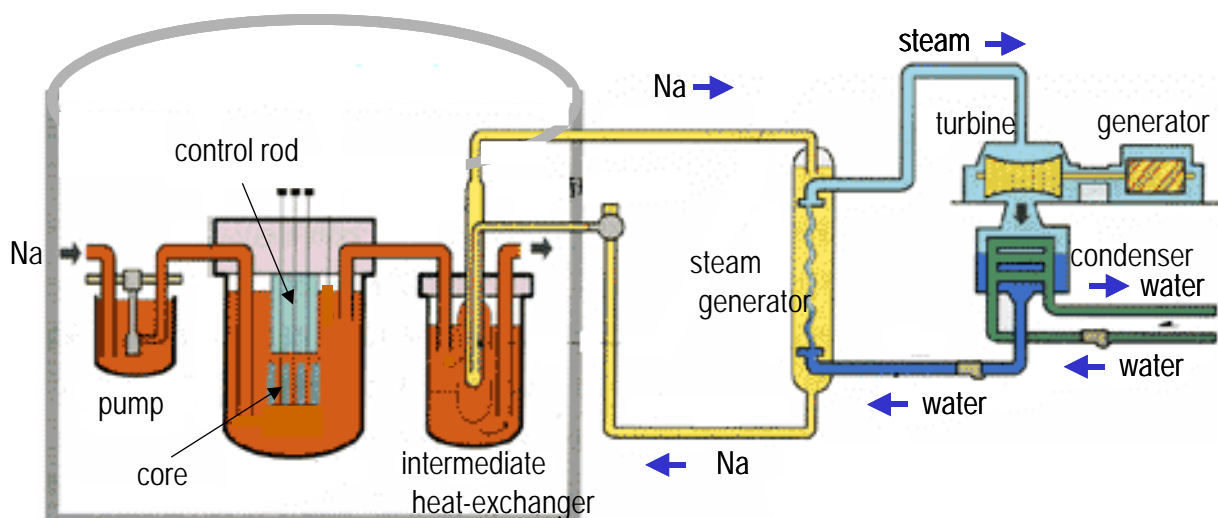
Figure 1.20   Fast breeder reactor (loop-type).

(1-5) Time-dependent Change of a Reactor and its Control

(1-5-1) Dynamic Characteristics of a Reactor

Denoting the effective multiplication factor as k_{eff}, the number of neutrons increases by k_{eff} after one generation. The average length of one generation is called the prompt neutron lifetime. Thermal reactors, in which fission takes place after neutrons are moderated, have much longer lifetimes than fast reactors, in which fission takes place without moderation. Nevertheless, the values are very small; the lifetime in a light-water reactor is $2-6 \times 10^{-5}$ sec, and is $0.8-2 \times 10^{-7}$ sec for a fast reactor. Denoting the lifetime as l, we can express the change in the number of neutrons as follows:

$$\phi(t) = \phi(0) \exp \left(\frac{k_{eff} - 1}{l} \right) \quad . \tag{1-38}$$

Here delayed neutrons are ignored. In the case of a slow light-water reactor of $l = 2 \times 10^{-5}$ sec, the number of neutrons increases by a factor of 150 in 1 second, even when $k_{eff} = 1.0001$. In the control of nuclear reactors, the amount by which the multiplication factor is different from 1 is important. Thus, the reactivity defined below is often used:

$$\rho = \frac{k_{eff} - 1}{k_{eff}} \quad . \tag{1-39}$$

For a change as rapid as mentioned above, it is impossible to control the chain reaction. In reality, however, the change becomes milder because of the contribution from delayed neutrons. Numerous kinds of fission products emit delayed neutrons, as mentioned in Secs. (2-6) and (3-3), and thus there are many kinds of decay constants. Normally they are handled in six groups, as shown in Table 1.8, where the decay constant is that of delayed neutron precursor and the yield is the fission product yield of the delayed neutron precursor multiplied by the delayed neutron yield of the precursor.

Table 1.8　Six group representation[3] of delayed neutrons in the thermal fission of ^{235}U.

Group (g)	Decay constant (λ_g, sec^{-1})	Yield (β_g)
1	0.0124	0.00053
2	0.0305	0.00355
3	0.111	0.00318
4	0.301	0.0064
5	1.14	0.00187
6	3.01	0.00068

If criticality cannot be maintained without the help of delayed neutrons, the number of neutrons can be maintained only after the contribution from delayed neutrons. Thus, the multiplication time of neutrons is controlled by the decay constants of the delayed neutron precursors. Compared with the above-mentioned prompt neutron lifetime l, the inverse of the decay constants are very large (for example, 81 seconds for group 1). Thus, the variation of the neutron flux is at a

speed that a person can easily control. This state is called a delayed critical state. A critical state that is achieved only with prompt neutrons is called a prompt critical state. Since delayed neutron yields are generally significantly smaller than 1, it is not easy to achieve a delayed critical state without the possibility of a prompt critical state. However, nuclear reactors are usually designed to satisfy this requirement.

The variation of the output power becomes of the order of seconds due to delayed neutrons, but control is still difficult. However, nuclear reactors generally have the following characteristic. If the output power increases, the reactivity becomes negative and the reactor tends to decrease the output power. If the output power decreases, the reactivity becomes positive and the reactor tends to increase the output power. In other words, the output of a nuclear reactor exhibits negative feedback. The magnitude of the feedback can be changed over a wide range by the design of the nuclear reactor. If a suitable negative value is adopted, control will become easy and the output power will stabilize. In Japan, positive feedback is prohibited by law. I will explain some important types of feedback below.

Reactor fuel contains fissile material and fertile material. The fertile material has large resonance absorption, as shown in Sec. (4-1) for ^{238}U. Because of this large absorption, the neutron spectrum (neutron flux) has a sharp dip at this energy. Therefore, the number of absorbed neutrons decreases compared to a flat neutron spectrum. This is called self-shielding. For a nuclear reactor, there are two important kinds of self-shielding; one was mentioned in Sec. (4-2) and the other is discussed here. If the output power and temperature increase, the thermal motion of fuel will intensify. Thus, when a neutron in motion with a constant energy E collides with a fuel nucleus, the energy should be modified by the thermal motion of the nucleus. This means that the resonance of the cross-section widens, while the area stays constant as shown in Figure 1.23. Thus, the peak of the cross-section decreases, the self-shielding effect is reduced, and absorption increases. This is clearly negative feedback for ^{238}U capture resonance, however, if the resonance reaction is a nuclear fission, it becomes positive feedback. This is called the Doppler effect. Here I explain the Doppler effect through spectral depletion by resonance reactions. It can also be explained though elementary neutron slowing-down history, which is also shown in Fig. 1.21.
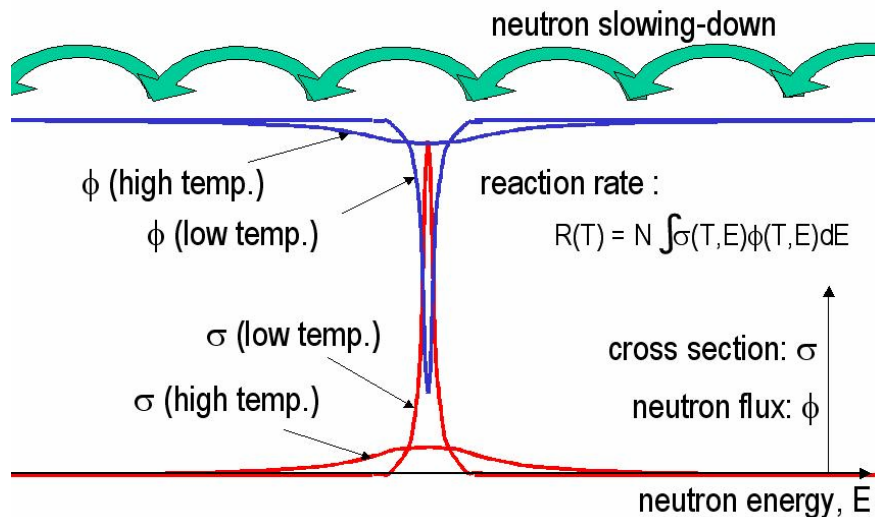

Figure 1.21   Doppler effect.

In a thermal reactor, fission is mainly due to thermal neutrons, which are approximately in

thermal equilibrium with the moderator. When the output power increases and the temperature of the moderator increases, the energy of the thermal neutrons also increases. This is called the thermal neutron spectral shift. In this case, there are various important cross-sections in the thermal neutron region, which change in a complicated manner with changes in energy. Thus, how the reactivity changes is a difficult question. However, negative feedback generally results because the nuclear fission cross-section decreases and neutron leakage from the core increases due to a decrease of the total cross-section.

The Doppler effect is related to the fuel temperature, and the thermal neutron spectral shift is dependent on the moderator. When there is power fluctuation, the Doppler effect initially applies, and then thermal neutron spectral shift occurs.

In addition, feedback applies to the output power through the expansion and deformation of the fuel, coolant, and moderator. Feedback also occurs through changes in the pressure and the voiding of the coolant and moderator. Here the void effect is generally treated by the void coefficient.

It is important to pay attention to the above effects if the output power is changed during operation or an accident happens. How the reactor changes when the output power is changed or an accident occurs is called the dynamics or kinetics of the reactor. Research that does not consider time-dependent changes is called statics.

(1-5-2) Effect of Xenon

In the preceding section, the dynamic characteristics of a reactor during a short period were described. When we consider the power fluctuation of a reactor over a longer period, the effect of xenon (^{135}Xe) is very important. The fission product ^{135}Xe has a large thermal neutron cross-section, and it greatly affects the reactivity control of the reactor.
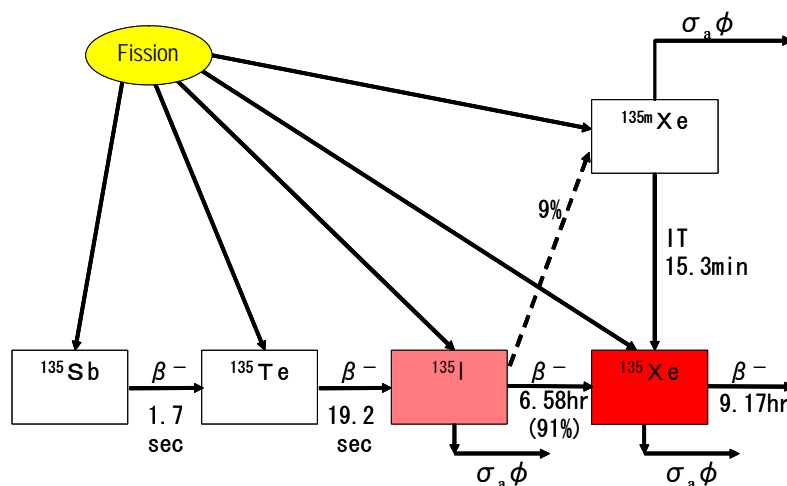
Figure 1.22   Fission products decay chain including ^{135}Xe.

The nuclide ^{135}Xe is generated in nuclear fission as shown in Fig. 1.22. If we approximate the effects of short-life nuclides, the change can be represented as shown in Fig. 1.23. Here γ is the fission product yield (yield of fission products generated per nuclear fission) and λ is the decay constant. The fission product yield and decay constant for ^{135}I and ^{135}Xe in the fission of ^{235}U are shown in Table 1.9. The fission product yields for other fissile materials are comparable.

From these results, we can see that the path for the formation of ^{135}Xe is as follows. Initially ^{135}I is formed by nuclear fission, then ^{135}Xe is formed by β-decay of ^{135}I with a half life of 6.58 hours.
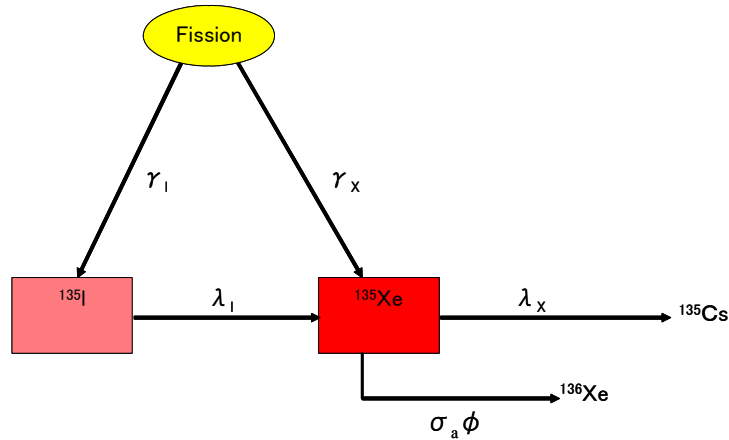
Figure 1.23   Approximation of fission products decay chain including ^{135}Xe.

Table 1.9   Fission product yield and decay constant for ^{135}I and ^{135}Xe in the fission of ^{235}U.

	Fission product yield (%)	Decay constant (hr^{-1})
^{135}I	6.3056	0.10485
^{135}Xe	0.2427	0.07634

This formation path essentially works as positive feedback for the reactor power output and is not desirable in reactor operation. That is, since the direct formation of ^{135}Xe by fission is very small, if the output power increases, ^{135}Xe will decrease because of an increase in absorption of neutrons, due, in turn, to an increase in the thermal neutron flux. Then, the decrease in the neutron absorber will increase the reactivity of the reactor and will further increase the neutron flux. However, this phenomenon will not continue indefinitely. The output power will ultimately decrease since ^{135}I, the amount of which increases because of the increase in the output power, becomes ^{135}Xe, hence increasing the amount of ^{135}Xe. When the output power decreases, a similar process takes place, that is, neutron absorption by ^{135}Xe decreases. However, the amount of ^{135}Xe derived from ^{135}I does not change much since the amount of ^{135}I does not change rapidly. Therefore ^{135}Xe increases as neutron absorption decreases, and thus the output power further decreases. This mechanism will generally cause a divergent oscillation in the output power.

When the output power is changed rapidly and to a great extent, for example, when the output power is rapidly decreased, ^{135}Xe will increase since the neutron flux decreases. In order to keep the reactor critical, it is necessary to withdraw the control rods. If the total neutron absorption capability of the control rods inside the core is smaller than the neutron absorption capability of the accumulated ^{135}Xe, the control rods inside the core must be completely withdrawn, and the reactor will then soon become subcritical. If the output power is increased beyond the total neutron absorption capability of the control rods, sufficient neutron absorber to counteract the decrease of ^{135}Xe cannot be inserted into the core and the output power will be out

of control. Therefore, restrictions are generally set for the power fluctuation range.

^{135}Xe works as positive feedback for the output power. Thus, it makes the output power unstable. However, since the half life of ^{135}Xe is sufficiently long, a small fluctuation can be easily controlled with control rods. Thus, it is possible to maintain the power at a constant output. Even though we can maintain the power of the total core at a constant output, spatial instability may be caused. That is, the output power at the upper part of the core increases and that at the lower part of the core decreases. If this happens, the output power at the upper part of the core further increases and that at the lower part of the core further decreases, because of the reason mentioned above. Thus, despite the constant total output power, the power distribution may become increasingly distorted. This phenomenon is called xenon oscillation. It is not as unstable as the oscillation of the total core; the change is much gentler, since neutrons diffuse from regions of high neutron flux to regions of low neutron flux. Among the various spatial modes, modes with weak coupling between peaks and valleys are more unstable. Modes with one peak and one valley are less stable than modes with many peaks and valleys. In addition, modes in which a peak and a valley are separated are less stable than modes in which a peak and a valley are close together. In a large reactor, coupling between peaks and valleys becomes weak, and thus xenon oscillation can more easily take place. This type of oscillation cannot be controlled without well-designed control rods, and it can cause reactor accidents. Xenon oscillation is significantly influenced by other power feedbacks mentioned in the previous section. If the other feedbacks are negative, xenon oscillation can be suppressed. In the case of a BWR, negative feedback due to the void is large, and therefore xenon oscillation is not significant. In the case of an ordinary PWR, negative feedback is not large, and therefore they are equipped with special control rods for the control of xenon oscillation.

(1-5-3) Burnup

The only naturally-occurring materials that can be used as nuclear fuel are uranium and thorium. The transformation of these materials in a nuclear reactor is shown in Figure 1.26. The letter m after the mass number shows a meta-stable state of the nucleus. Natural uranium contains ^{238}U and ^{235}U as main components and thorium contains only ^{232}Th. Here ^{235}U is the only fissile material; ^{238}U and ^{232}Th are fertile materials. ^{239}Pu and ^{241}Pu are the main fissile materials generated from ^{238}U, and ^{233}U is the main fissile material from ^{232}Th. Since the fission cross section for some fissile nuclides is dominantly high but not so dominant for others, the definition of fissile in Fig. 1.24 is not definitive.

Although the amount of the fertile materials ^{238}U and ^{232}Th decrease with the progress of burnup, they can be considered constant in the first approximation. The amounts of the daughter nuclides increase with the progress of burnup. However, all important nuclides have specific characteristics that lead to their eventual saturation. These characteristics are due to neutron absorption and decay, and the nature of the saturation value depends upon whether the decrease of the nuclide is due to neutron absorption or decay. For example, the decrease of ^{239}Pu due to decay is considered to be zero and thus its saturation value does not depend upon the neutron flux level. At the neutron level of presently operated nuclear reactors, the decrease of ^{233}Pa, which is generated by the neutron absorption of ^{232}Th, is predominantly due to decay. Thus, the saturation value is proportional to the neutron flux level. The same can be said for fission products. The saturation value for ^{149}Sm is proportional to the neutron flux level. However, when the saturation value is proportional to the neutron flux level at a normal output power level, it may be that the saturation value does not depend upon the neutron flux level if the output power increases.

(a) From thorium   (b) From uranium
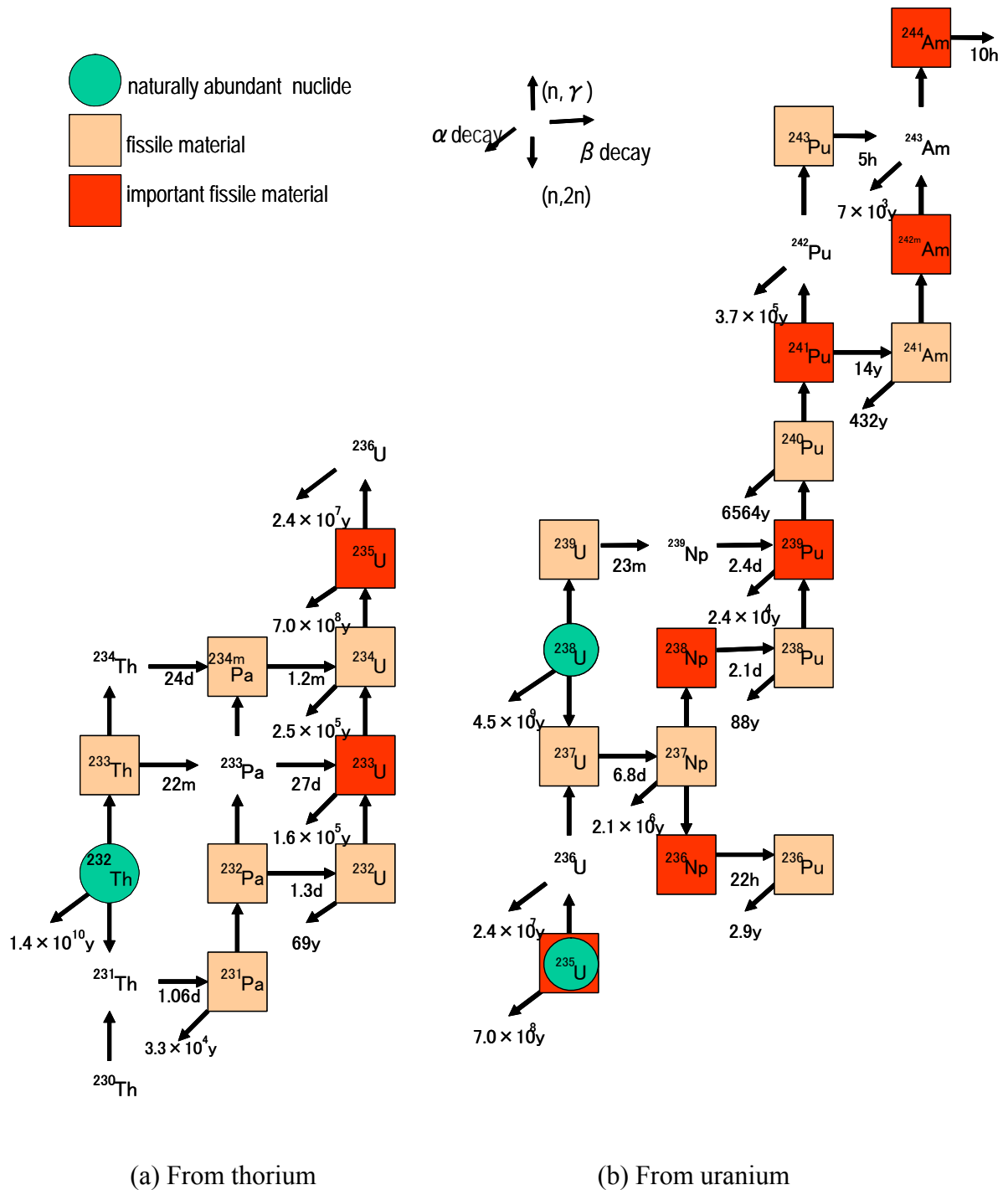
Figure 1.24   Actinide chain from nuclear fuel in nuclear reactor.

The reactivity when all control material is removed from the core is called the excess reactivity. Generally, the excess reactivity changes with the progress of burnup as shown in Fig. 1.25. If the enrichment of loaded fuel increases, the initial excess reactivity becomes large and thus higher burnup can be achieved. Here, burnup is defined as the amount of obtained energy per unit fuel. However, the conversion ratio deteriorates because of decreased absorption by the fertile material, and fission products accumulate with the progress of burnup. Therefore, burnup

does not greatly increase in spite of increased reactivity. Initially the excess reactivity rapidly decreases, as shown in the figure. This is due to the increase in the temperature and the accumulation of xenon. However, the curve of the excess reactivity soon becomes upwardly convex, the main reason for which is the saturation of the accumulation of [239]Pu, which has a larger fission cross-section than [235]U.
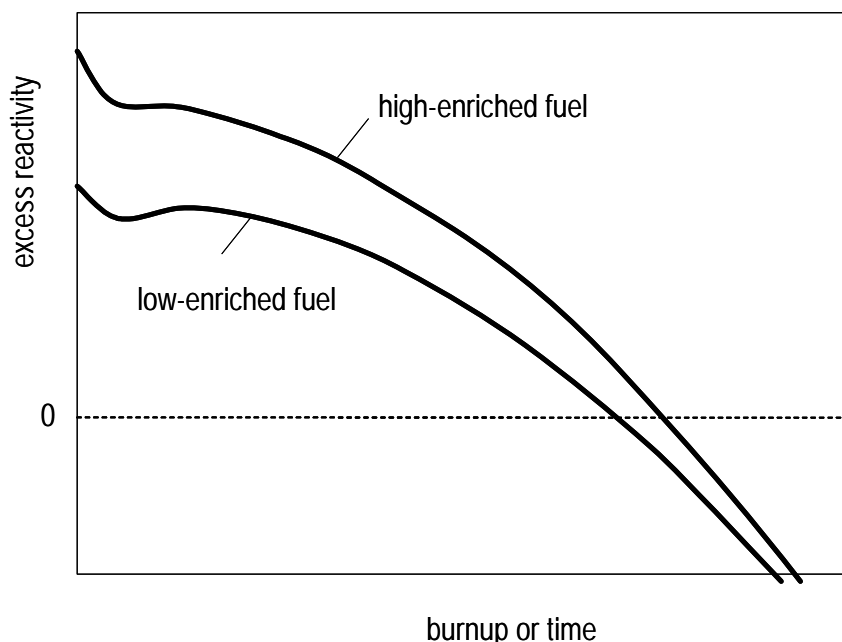
Figure 1.25　Excess reactivity change during burnup.

　　　The excess reactivity for one-batch burnup without refueling changes as shown in Fig. 1.26. If we separate the batch into two, the following takes place: In Fig. 1.26, we burn the fuel for a time t, with $t_1=t_2=t$ and $\rho_1=\rho_2$. The batch that has burned more is then replaced with fresh fuel. In this way, the burnup is stretched up to e_2, which is larger than e_1. In addition, the initial excess reactivity of the reactor decreases from ρ_0 to $(\rho_0+\rho_1)/2$. This is ideal in that we can decrease waste neutrons, which are absorbed by the control material. It is also an advantage for reactor safety. The more we increase the number of batches, the more the burnup can be improved. If the number of batches is infinite, the burnup can be increased up to e, at which point the two shaded areas in the figure become equal. Under this condition, the reactor is always critical and control material for burnup compensation is not necessary. Here we have assumed that the importance of all batches is the same (where the importance is the degree of the effect on the multiplication factor of the entire reactor by in situ generated neutrons). If a fuel with smaller burnup, namely, a fuel with larger reactivity, is located at the place where the importance is high, burnup of the fuel can be further increased. However, this is not desirable since the power peaking (maximum power density/average power density) becomes large. Instead the reverse is practiced in order to flatten the output power. In light-water reactors, typical of nuclear reactors, three or four batches are generally used, and the fuel is changed every year at the time of regular inspections. For the first cycle, the fuel is all new, and thus the excess reactivity becomes too large if the enrichment is the same for all the fuels. Therefore, in a reactor in which enriched uranium is used, the enrichment is changed for different batches and fuel replacement begins from the lowest enrichment batch. Even if the initial reactivity is adjusted to that of the equilibrium cycle by this method, [239]Pu is accumulated in the first cycle and the time necessary for the excess reactivity to

become zero is longer than in the equilibrium cycle. Therefore, the first cycle is sometimes made longer than the later cycles. Specific properties generated in the first cycle are propagated, in various ways, to the later cycles and cause handling problems.
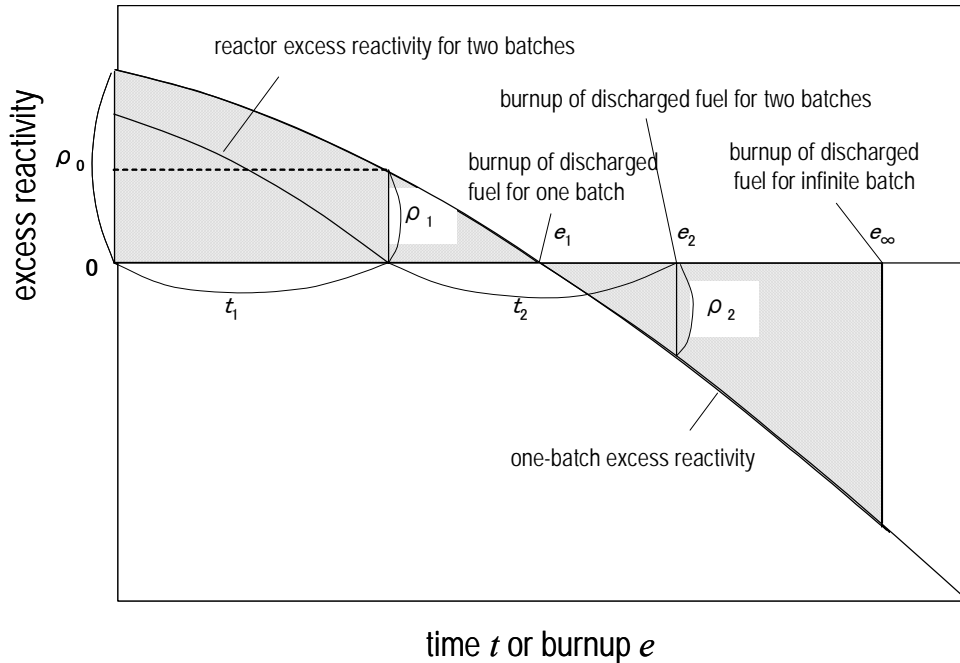

Figure 1.26   Excess reactivity change during burnup.

Merely increasing the number of batches (to 3 or 4) is not satisfactory since the initial excess reactivity of the reactor is still rather high. Suppressing this excess reactivity only with control rods is not ideal from the viewpoint of safety and possible distortion of the power distribution. Usually, to suppress the excess reactivity, a material with a large absorption cross-section that decreases faster than the decrease of the reactivity is uniformly distributed so that a desirable power distribution is obtained in the reactor. This type of material is called burnable poison, examples of which are ^{10}B and Gd. Their cross-sections are shown in Figure 1.14. When the decrease of the reactivity is rapid, Gd with a large cross-section can be used. However, since the absorption cross-section of Gd has a resonance in the thermal region, it may give a positive temperature coefficient, and thus care should be taken in its use. Desirable burnable poison suppresses the excess reactivity as much as possible and is consumed at the end of the cycle. As shown in Fig. 1.24, the curve of the excess reactivity is a straight line or a mildly upwardly convex curve. However, the neutron absorber generally decreases as $\exp(-\sigma_a t)$, which cannot compensate the curve of the excess reactivity. Therefore, self-shielding, which was mentioned in Sec. (4-1), is utilized. That is, burnable poison is heterogeneously formed and absorption is suppressed by self-shielding at the beginning of the cycle. At the end of the cycle, there is no self-shielding and absorption is promoted. The curve for the decrease of burnable poison becomes convex downward when the number of burnable poison isotopes is increased. Therefore, handling is usually easier if the number of isotopes is small. Since the curve of the excess reactivity is different in each cycle, it is necessary to appropriately adjust the excess reactivity. As described later, spatial adjustment is also important. If the initial amount of poison is too small at a certain section, the output power of that section will become too large and the poison will rapidly decrease. Thus, with the progress of burnup, the design standard for the power

peaking may be surpassed. Precautions are therefore necessary.

The portion of the reactivity that cannot be compensated by the above methods is compensated by the control material. As control material, ^{10}B, Hf, and Cd are used. The cross-sections for these materials are shown in Figure 1.14. Because of its positive temperature coefficient and other material issues, Cd is used as an alloy of Ag and In. ^{10}B is mixed with iron or stainless steel, and is also used as compounds such as carbide. These control materials are normally used in the form of rods. According to the Haling principle, concerned with the operation method of control rods, the best operation is to keep the power distribution constant during a cycle. At the end of the cycle, the power distribution cannot be changed by control rods since all the control rods have been withdrawn. Therefore, in order to operate according to the Haling principle, the power distribution at the end of the cycle should be created at the start of the cycle and maintained during the cycle by properly using control rods. However, with a finite number of control rods, this is impossible. In contrast, since the excess reactivity to be suppressed is too large, the power peaking at the beginning of the cycle becomes a maximum (however, if the axis direction is also taken into account, it is generally larger when the control rods are half inserted). The number of control rods and the design is decided by considering how the power peaking can be suppressed and maintained within the reactor design limit. Thus, operation with control rods results in large power peaking. Therefore, in PWR and heavy-water reactors, boric acid is mixed into the moderator and the concentration is adjusted during the operation. In this way, large power peaking can be avoided since boric acid is uniformly distributed in the moderator.

(1-5-4) Fuel Management

For acceptable power peaking, not only the control material but also the fuel arrangement in the reactor is very important. The type of fuel used and how it is arranged in the core are issues of fuel management. Since the management of the entire fuel cycle, including enrichment, fabrication, reprocessing, and disposal, which is separate from the reactor, is also called fuel management, fuel management in the present case is often specifically called in-core fuel management. Fuel management in the reactor depends upon the types of nuclear reactor. Here I will explain some characteristics of water reactors, high-temperature gas-cooled reactors, and fast reactors.

Along the direction of the coolant channel, the situation changes depending on the design constraint of the fuel element. In a high-temperature gas-cooled reactor, maximum center temperature restriction in the fuel particle is most effective. In order to satisfy this, fuel with a larger reactivity is arranged near the coolant channel entrance. Thus, we allow the power to approach an exponential distribution, taking large values near the coolant channel entrance to flatten the maximum fuel center temperature. On the other hand, in a water reactor in which a liquid is used for cooling, the easier the coolant boils, the more effective the heat flux restriction due to burnout. In this case, a flat power distribution is better. Even when an interaction between the cladding tube and fuel pellet exists and burnup restrictions apply, the power should be flat. However, a flat distribution is unstable under perturbations. When the fuel distribution is uniform, the power distribution approaches a cosine distribution and is more stable under perturbations. The cosine distribution flattens during fuel burnup.

In a reactor, a flat power distribution along the direction perpendicular to the coolant channel is better, since a greater output power can be obtained. In this case though, a flat distribution tends to be unstable. However, in the normal control rod design, control is easier along this direction than along the coolant channel axis. The power distribution along this direction is closely related to the refueling system, which varies widely depending upon reactor type. A light-water reactor has a small core and it is easy to reassemble the entire fuel at each

40

cycle. Therefore, there is considerable freedom in the fuel arrangement. Questions of how refueling should be performed throughout the life of the reactor which include multiple recycles and how the fuel should be arranged have been studied using simple modeling of the core by various methods and very complicated solutions were obtained. These results themselves cannot be applied as they are to actual reactors because of modeling restrictions. However, they support the empirical "out-in + scattering system" in which fresh fuel should be preferably placed at the outside of the fuel region and fuel with different burnup should be uniformly mixed and preferably placed inside. A mathematical method using the empirical rule is under investigation for application to an actual light-water reactor.

Since their core structures are similar, the fuel loading methods for fast reactors and light-water reactors are not very different. However, the fuel loading method for heavy-water reactors and high-temperature gas-cooled reactors are significantly different. The core size per unit power is much larger for heavy-water reactors and high-temperature gas-cooled reactors than for light-water reactors. However, refueling under operation is actively adopted for these larger reactors. If continuous refueling under operation is possible, neutron absorber to suppress excess reactivity is not necessary. Thus, the neutron economy improves and an increase in the conversion ratio or burnup is possible. In addition, that the core has little neutron absorber means that accidents due to increased reactivity by ejection of the neutron absorber from the core are avoidable, which is very desirable from the point of view of safety .

(1-5-5) Nuclear Equilibrium State

What ultimately happens if the fuel is burnt continually with continuous supply of uranium or thorium and with continuous discharge of fission products?

As plutonium is generated from uranium by neutron absorption, if the fuel keeps absorbing neutrons, either nuclear fission will take place, or the atomic number of a nuclide will increase by β-decay since the neutron number becomes too large. Thus, nuclear fuel that has repeatedly absorbed neutrons without nuclear fission taking place will keep increasing its atomic number. However, it soon becomes a nuclide with a short α-decay life and the atomic number will then decrease by α-decay. By this mechanism, if fuel is left in the reactor and fresh fuel is supplied only for the portion of fuel lost through fission, the isotope composition of the fuel in the reactor reaches an equilibrium state.

The nuclide number densities in the equilibrium state are shown in Fig. 1.27 for a sodium-cooled oxide-fuel fast reactor and a light-water reactor, when natural uranium or thorium is loaded as fresh fuel. The nuclide number density spectrum when thorium is loaded is shifted to smaller atomic numbers by 2 relative to the spectrum when natural uranium is loaded. The fast reactor shows high densities of directly generated fissile nuclides compared with the thermal reactor, but they rapidly decrease as the mass number increases. Accordingly, the fast reactor is easily made critical and generates less higher actinides.

The nuclide density obtained with natural uranium supply for fast reactor shows highest performance of criticality, but for thermal reactor impossible to realize criticality. The thorium fuel supply can realize criticality for both thermal and fast reactors, but better for fast reactor.
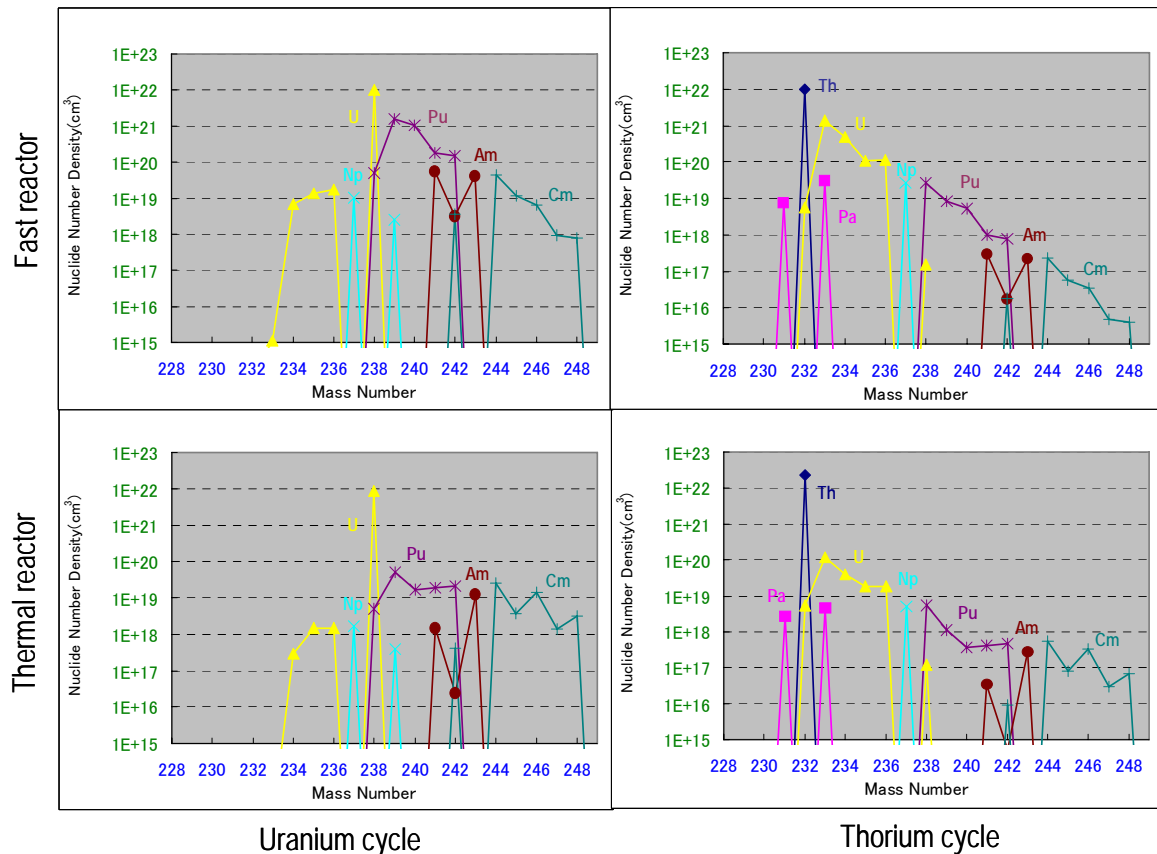
Figure 1.27 Nuclide number densities in the equilibrium state
for different neutron spectra and different loaded fuels. [4]

(1-5-6) Fuel Cycle

So far I have described the use of fuel in a nuclear reactor. This fuel is fabricated in the following way. Mined uranium and thorium are processed and the uranium is sometimes enriched. They are then fabricated into fuel assemblies and loaded into the reactor. Spent fuel, which has become useless, is removed from the reactor to be reprocessed or disposed. This is called the fuel cycle. However, since it is outside the scope of this course, a detailed explanation will be omitted here.

Fuel removed from the nuclear reactor still contains residual uranium or newly generated plutonium, which can be reused as fuel. From the spent fuel, fissile material can be extracted, reprocessed as fuel, and used again in a nuclear reactor, a process called recycling. Spent fuel may be disposed as it is, and a cycle in which this is done is called a once-through cycle.

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[1] You can get the data from <http://ie.lbl.gov/toimass.html>.
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Though there are many textbooks on nuclear reactor theory, but only few books are referenced for each category here to avoid laborious selection works of students.

(1) Nuclear reactor in general
(1-1) R. L. Murray, "Nuclear Energy, 5th ed.," Butterworh Heinemann, Boston (2001).
(1-2) J. R. Lamarsh and A. Baratta, "Intro. to Nuclear Engineering, 3rd ed.," Prentice Hall Inc., New Jersey (2001).
(1-3) S. Glasstone and A. Sesonske, "Nuclear Reactor Engineering, 3rd. ed.," Van Nostrand Reinhold Co., New York (1981).

(2) Reactor physics in general
(2-1) J. J. Duderstadt and L. J. Hamilton, "Nuclear Reactor Analysis," John Wiley and Sons, Inc., New Yourk (1976).
(2-2) J. R. Lamarsh, "Intro. to Nuclear Reactor Theory," Addison-Wesley Pub. Co., Reading, Massachusetts (1966).

(3) Reactor physics analysis
(3-1) G. I. Bell and S. Glasstone, "Nuclear Reactor Theory," Van Nostrand Reinhold Co., New York (1970).
(3-2) M. Clark, Jr. and K. F. Hansen, "Numerical Methods of Reactor Analysis," Academic Press, New York (1964).
(3-3) S. A. Dupree and S. K. Fraley, "A Monte Carlo Primer," Kluwer Academic/Plenum Pub., New York (2002).
(3-4) K. Kobayashi, "Nuclear Reactor Theory," Corona Pub.Co., Tokyo (1996) (written in Japanese)

(4) Reactor dynamics
(4-1) D. L. Hetrick, "Dynamics of Nuclear Reactors," American Nuclear Society, La Grange Park, Illinois (1993).

(5) Burnup and fuel management
(5-1) H. W. Graves, Jr., "Nuclear Fuel Management," John Wiley and Sons, New York (1979).

(6) Early history
Various interesting history books have been published. However, I think the following one is excellent.
(6-1) R. Rhodes, "The Making of the Atomic Bomb", Simon & Schuster, New York (1986).
This book has received a Pulitzer Prize. Translated book under the title "Genshi Bakudan No Tanjou" is sold by Kinokuniya Bookstore (1995). In addition, the sequel "Dark Sun: The Making of the Hydrogen Bomb" by the same author has been published (1995).

Part 2
Reactor Analysis

Introduction

In Part 1 "Elements of Nuclear Reactor Theory", we studied an overview of nuclear reactors and how nuclear energy is extracted from reactors. Here, nuclear energy means the energy released in nuclear fission. This occurs because of the absorption of neutrons by fissile material. Neutrons are released by nuclear fission, and since the number of neutrons released is sufficiently greater than 1, a chain reaction of nuclear fission can be established. In turn, this allows energy to be extracted from the process. The amount of extracted energy can be adjusted by controlling the number of neutrons. The higher the power density is raised, the greater the economic efficiency of the reactor. The energy is extracted usually as heat via the coolant circulating in the reactor core, and finding the most efficient way to extract the energy is a critical issue. The higher the coolant output temperature is raised, the greater the energy conversion efficiency of the reactor. Considerations of material temperature limits and other constraints make a uniform power density desirable. Ultimately, this means careful control of the neutron distribution. If there is an accident in a reactor system, the power output will run out of control. This situation is almost the same as an increase in the number of neutrons. Thus, the theory of nuclear reactors can be considered the study of the behavior of neutrons in a nuclear reactor. The behavior of neutrons in a nuclear reactor will be described in Part 2.1 "Transport Equation and Diffusion Equation", which is a basis of Part 2 "Reactor Analysis".

Note that the two terms used here, "nuclear reactor theory" and "reactor analysis", are used to mean nearly the same thing. The terms "reactor physics" is also sometimes used. This field addresses the transport, moderation (slowing-down), and diffusion of neutrons. However, with the development of the analysis of nuclear reactors, especially light water reactors, this field has taken on many facets. The treatment in this textbook is not limited to light water reactors, but is intended to summarize the general knowledge about neutron transport.

First, a formulation will be developed for neutron transport. The derivations have been simplified as much as possible. This presentation was chosen because we believe that it is more effective to derive the equations directly, without a text.

There are many ways to solve the equations that follow. Here, we derive the diffusion equation, and then we present a simple method for solving the equation analytically, along with a discussion of numerical solutions. Methods for finding the coefficients of the diffusion equation are also important, but since much space would be necessary to cover even a single method – and many such methods are currently employed – this topic is not addressed here.

Finite-difference methods including the S_N method and the Monte Carlo method are used to solve the transport equation. These are important topics, but to save lecture time, they are also not treated here. In the future, we may introduce them in the lectures.

Time-dependent problems will be incorporated into the text once they have been organized from the lecture notes.

Part 2.1
Transport Equation and Diffusion Equation

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(2-1-1) Introduction

It is essential to know the spatial and energy distributions of the neutrons in a field in a nuclear fission reactor, D–T (or D–D) fusion reactor, or other nuclear reactors populated with large numbers of neutrons. It is obvious why the spatial distribution should be known, and because neutron reactions vary widely with energy, the energy distribution is also a critical parameter. The neutron energy distribution is often called the *neutron spectrum*. The neutron distribution satisfies transport equation. It is usually difficult to solve this equation, and often approximated equation so called diffusion equation is solved instead. In Part 2.1 only overview of transport equation and diffusion equation of neutrons are presented, and methods for solving these equations are presented in the following parts. Numerical analysis of diffusion equation is given in Part 2.2.

(2-1-2) Neutron Density and Flux

The neutron distribution is expressed by several quantities. The number of neutrons n in unit-volume at location r, moving in direction Ω per unit-solid angle with energy E at time t, or $n(r,\Omega,E,t)$, is called the *neutron angular density*. If the number of neutrons with a given energy is counted per unit volume, without respect to the direction of travel, the *neutron density* is obtained:

$$n(r, E, t) \equiv \int_{4\pi} n(r, \Omega, E, t) d\Omega \ . \tag{2-1-1}$$

When the neutron density is integrated across the energy range, the *total neutron density* is obtained:

$$n(r, t) \equiv \int_0^\infty n(e, E, t) dE \ . \tag{2-1-2}$$

Both the neutron angular density and the total neutron density are sometimes simply called the *neutron density*, so the reader must take care to distinguish from the context which meaning is intended.

When the neutron density in a specific direction is multiplied by the neutron speed v, the *neutron angular flux* is obtained:

$$\phi(r, \Omega, E, t) \equiv vn(r, \Omega, E, t) \ . \tag{2-1-3}$$

When the direction is disregarded and the neutron density is multiplied by v, the *neutron flux* or – to distinguish it from the above – the *scalar neutron flux* is obtained:

$$\phi(r, E, t) \equiv vn(r, E, t) \ . \tag{2-1-4}$$

This can also be defined as the sum of the neutron traces passing through a sphere of unit radius over a unit time. The sum of the neutron flux over all energies is called the *total neutron flux*:

$$\phi(r, t) \equiv \int_0^\infty \phi(r, E, t) dE \ . \tag{2-1-5}$$

Note that both the neutron angular flux and the total neutron flux are often simply called the *neutron flux*, so the reader must take care with this term. The symbols ϕ and n are used for several different definitions, but note that the dimensions and values are naturally different for the different definitions.

originating in nuclear fission.
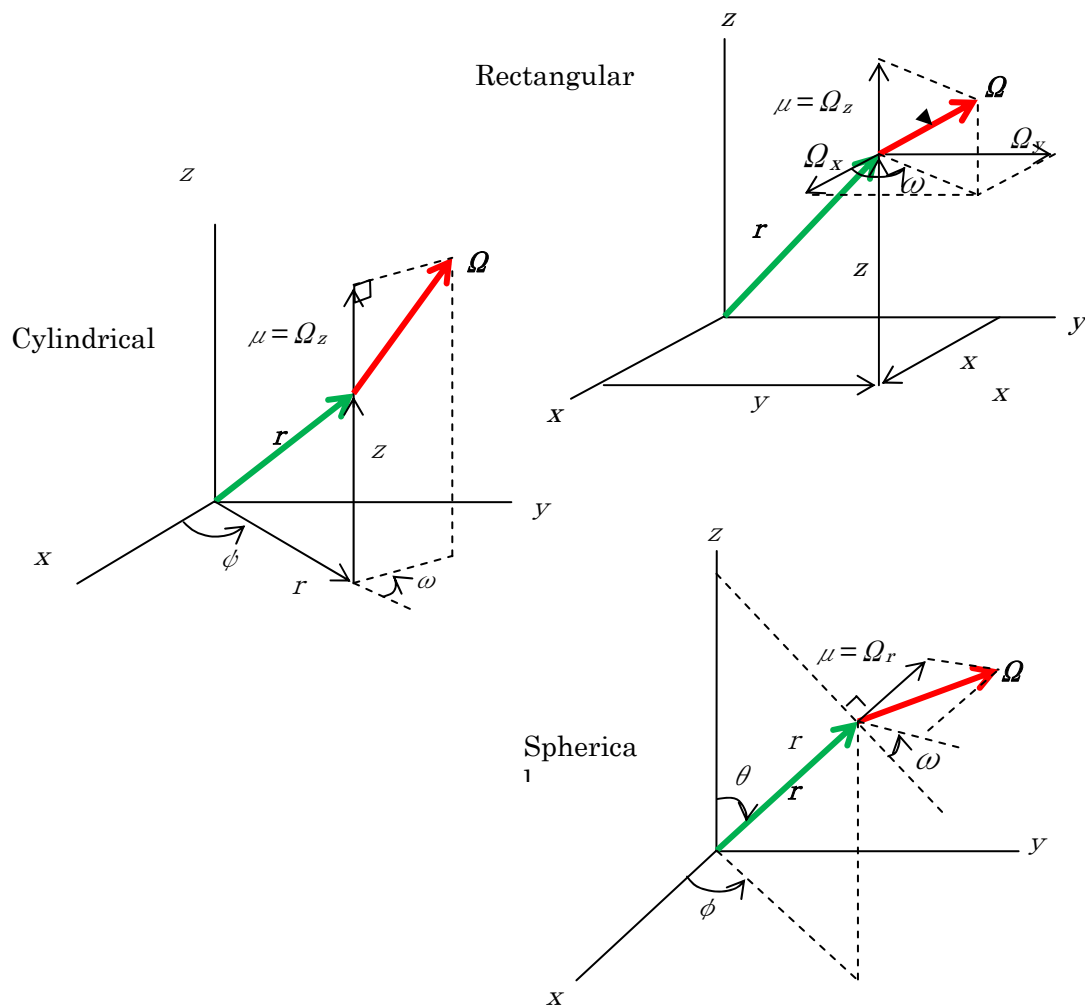
Figure 2-1-1   Typical coordinate systems used for neutron transport equation.

Table 2-1-1   Forms for $\Omega \cdot \nabla$ and $\int_{4\pi} d\Omega$ in typical geometries.

$$\Omega \cdot \nabla \qquad\qquad\qquad\qquad\qquad\qquad \int_{4\pi} d\Omega$$

Infinite flat plane: $(x\ ;\mu)$

$$\mu \frac{\partial}{\partial x} \qquad\qquad\qquad\qquad\qquad\qquad 2\pi \int_{-1}^{1} d\mu$$

Rectangular: $(x,\ y,\ z\ ;\mu,\omega)$

$$\eta(\cos\ \omega\ \frac{\partial}{\partial x} + \sin\ \omega\ \frac{\partial}{\partial y}) + \mu \frac{\partial}{\partial z} \qquad\qquad \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\omega$$

Spherical (spherical symmetry): $(r\ ;\mu)$

$$\mu \frac{\partial}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial}{\partial \mu} \qquad\qquad\qquad 2\pi \int_{-1}^{1} d\mu$$

Spherical (general): $(r;\theta,\varphi;\mu,\omega)$

$$\mu \frac{\partial}{\partial r} + \frac{\eta}{r} \cos\ \omega\ \frac{\partial}{\partial \theta} + \frac{\eta}{r} \frac{\sin\ \omega}{\sin\ \theta} \frac{\partial}{\partial \phi} \qquad \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\omega$$

$$+ \frac{1-\mu^2}{r} \frac{\partial}{\partial \mu} - \frac{\eta}{r} \sin\ \omega\ \cot\ \theta\ \frac{\partial}{\partial \omega}$$

Cylindrical (infinite cylinder, axial symmetry): $(r\ ;\mu,\omega)$

$$\eta \cos\ \omega\ \frac{\partial}{\partial r} - \frac{\eta}{r} \sin\ \omega\ \frac{\partial}{\partial \omega} \qquad\qquad \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\omega$$

Cylindrical (general): $(r,\ z,\varphi;\mu,\omega)$

$$\eta \cos\ \omega\ \frac{\partial}{\partial r} + \mu \frac{\partial}{\partial z} + \frac{\eta}{r} \sin\ \omega (\frac{\partial}{\partial \phi} - \frac{\partial}{\partial \omega}) \qquad \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\omega$$

See Fig. 2-1 for explanation of symbols.

Table 2-1-1 provides specific forms for $\Omega \cdot \nabla$ and $\int_{4\pi} d\Omega$ in the typical coordinate systems shown in Figure 2-1-1.

For brevity, no explanation is given above for the derivation of Eq. (2-1-6). Several derivations have been formulated. In this textbook a hint for a derivation is given in Fig. 2-1-2. It may be clear to the reader how to proceed after considering the figure.

$$\left(\frac{1}{v}\frac{d}{dt} + \Omega \cdot \nabla + \Sigma_t \right) \phi(r,\Omega,E,t) = q$$
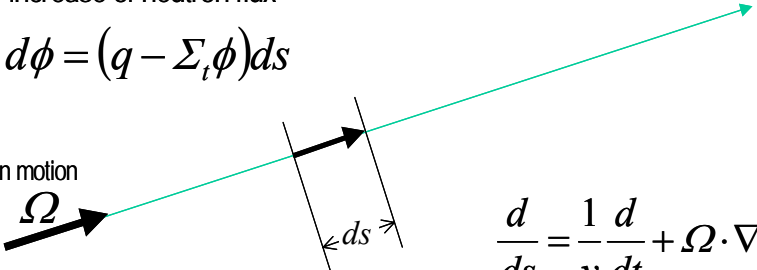
Neutron source

$$q(r,\Omega,E,t) = \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma(r,E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(r,\Omega',E',t) + S(r,\Omega,E,t)$$

Differential increase of neutron flux

$$d\phi = (q - \Sigma_t \phi)ds$$

Direction of neutron motion

$$\Omega$$

$$\frac{d}{ds} = \frac{1}{v}\frac{d}{dt} + \Omega \cdot \nabla$$

Figure 2-1-2   Differential picture of the transport equation

The line shows the neutron path. We choose a coordinate system s on this path to show the neutron position. You can derive the equation for transferring coordinate system from s to (t, r) easily as the following:

$$\frac{d}{ds} = \frac{dt}{ds}\frac{d}{dt} + \frac{dx}{ds}\frac{d}{dx} + \frac{dy}{ds}\frac{d}{dy} + \frac{dz}{ds}\frac{d}{dz}$$

$$= \frac{1}{v}\frac{d}{dt} + \Omega_x \frac{d}{dx} + \Omega_y \frac{d}{dy} + \Omega_z \frac{d}{dz}$$

$$= \frac{1}{v}\frac{d}{dt} + \Omega \cdot \nabla$$

If you consider the neutron balance in the differential distance ds on this path, you can derive the neutron transport equation.

Equation (2-1-6) is called the differential–integral expression of the transport equation. The neutron transport equation can also be given in the following integral form:

$$\phi(r,\Omega,E,t) = \int_0^\infty \exp[-\int_0^s \Sigma_t(r - s'\Omega, E)ds'] \times q(r - s\Omega, \Omega, E, t - \frac{s}{v})ds \qquad (2\text{-}1\text{-}12)$$

The derivation of this equation should be clear on examination of Fig. 2-1-3.

$$\phi(r,\Omega,E,t) = \int_0^\infty \exp\left[-\int_0^s \Sigma_t(r-s'\Omega,E)ds'\right] q(r-s\Omega,\Omega,E,t-\frac{s}{v})ds$$

Neutron source

$$q(r,\Omega,E,t) = \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma(r,E'\to E,\Omega'\to\Omega)\phi(r,\Omega',E',t) + S(r,\Omega,E,t)$$

Attenuation factor

$$\exp\left[-\int_0^s \Sigma_t(r-s'\Omega,E)ds'\right]$$

s

$$\phi(r,\Omega,E,t)$$

Direction of neutron motion

Ω

$$q(r-s\Omega,\Omega,E,t-\frac{s}{v})$$

Figure 2-1-3 Integral picture of the transport equation

The line also shows the neutron path. The neutron flux on the path and the coordinate of s is evaluated from only the neutrons on the path whose coordinate is less than s. The integral neutron transport equation shows this relation.

It is less common to directly solve the integral form than the differential–integral form, but since the theoretical interpretation of this form is easier, it is often used for theoretical development and interpretation. Its employment is especially preferred for theoretical study on the Monte Carlo method.

Due to the capabilities of computers, the general form of the transport equation is currently handled only by the Monte Carlo method. This solves the equation by numerical simulation of the movement of each neutron. The results are provided as statistical quantities, and hence the more histories taken, the smaller the statistical error in the results. The problem is obtaining statistically precise results in short calculation times. It is generally impossible to find $\phi(r,\Omega,E,t)$ itself with acceptable accuracy with this method; it is more suited for finding integrated values.

Below, the use of methods other than Monte Carlo for solving this equation is described.

(2-1-4) Slowing-down of Neutrons

(2-1-4-1) Continuous Energy Model

The transport equation in its general form is too difficult to handle directly, so initially we will address just the energy variables. For a steady-state neutron distribution in a uniform, infinite system, the transport equation (2-1-6) takes the following form:

$$\Sigma_t(E)\phi(E) = \int_0^\infty \Sigma(E' \to E)\phi(E')dE' + S(E) \quad . \tag{2-1-13}$$

The energy decreases during slowing-down. When handling this circumstance, it is often useful to use the *lethargy*, which increases with neutron slowing-down, in place of energy:

$$u = \ln(E_0 / E) \quad . \tag{2-1-14}$$

Here, E_0 is a selected standard energy value. Equation (2-1-13) can be rewritten as follows using u:

$$\Sigma_t(u)\phi(u) = \int_0^\infty \Sigma(u' \to u)\phi(u')du' + S(u) \quad . \tag{2-1-15}$$

This is a type 2 Fredholm integral equation and can be solved with a Neumann series as follows:

$$\phi(u) = \frac{S(u)}{E_t(u)} + \frac{1}{\Sigma_t(u)} \int_0^\infty \frac{\Sigma(u' \to u)}{\Sigma_t(u')} S(u')du'$$
$$+ \frac{1}{\Sigma_t(u)} \int_0^\infty \frac{\Sigma(u' \to u)}{\Sigma_t(u')} \int_0^\infty \frac{\Sigma(u'' \to u')}{\Sigma_t(u'')} S(u'')du'du'' + \cdots \quad . \tag{2-1-16}$$

The first term in the above is the direct contribution from the neutron source, the second term is the contribution from the first collisions by the neutrons, and, in general, the nth term is the contribution of the $(n-1)^{th}$ collisions.

When a neutron has low energy (conventionally, less than 100 eV), scattering occurs by means of S waves, and hence is only elastic scattering and is isotropic with respect to the center of mass system. In this case,

$$\Sigma(E' \to E) = \begin{cases} \dfrac{\Sigma_S(E')}{(1-\alpha)E'} & \text{for } \alpha E \le E \le E \\ 0 & \text{all other cases} \end{cases} \tag{2-1-17}$$

Rewriting this in terms of lethargy, we obtain:

$$\Sigma(u' \to u) = \begin{cases} \dfrac{\exp(u'-u)}{1-\alpha}\Sigma_S(u'), & \text{for } u' \le u \le u' + \varepsilon \\ 0 & \text{all other cases} \end{cases} \tag{2-1-18}$$

where Σ_S is the macroscopic scattering cross section and α is given by:

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 \qquad . \tag{2-1-19}$$

Here, A is the atomic mass in units of neutron mass, which is about the same as the mass number. ε is the maximum increase in lethargy at an elastic scattering and is given by:

$$\varepsilon = \ln(1/\alpha) \tag{2-1-20}$$

For a medium composed of a single kind of atom, when elastic scattering by S waves is the only mechanism for slowing-down, Eq. (2-1-15) can be described by the following:

$$\Sigma_t \phi(u) = \int_{u-\varepsilon}^{u} \Sigma_S(u')\phi(u')\frac{\exp(u'-u)}{1-\alpha}du' + S(u) \tag{2-1-21}$$

When there is no absorption, the delta function can be applied:

$$S(u) = \delta(u)$$

In this case, the solution is called the *Placzec function* as follows:

$$F_p(u) = \Sigma_S(u)\phi(u) \tag{2-1-22}$$

It has a discontinuity at $u = \varepsilon$. The first differential coefficients have a discontinuity at $u = 2\varepsilon$, the second differential coefficients have a discontinuity where $u = 3\varepsilon$, and so on. When u is very large, it approaches a constant:

$$F_p(u) = \Sigma_S(u)\phi(u) \fallingdotseq \frac{1}{\xi} \tag{2-1-23}$$

Here, ξ is the mean lethargy gained by a neutron in a single collision, and is obtained by the following:

$$\xi = 1 - \frac{\alpha\varepsilon}{1-\alpha} \tag{2-1-24}$$

(2-1-4-2) Multigroup Energy Model

The most commonly used techniques for numerically solving Eqs. (2-1-13) and (2-1-15) involve digitizing the energy variables and lethargy variables. The most common of these techniques is the multigroup method. Let us take Eq. (2-1-15) as an example. First, the lethargy is divided into groups (energy groups). Equation (2-1-15) then takes the following forms:

$$\Sigma_{t,g}\phi_g = \sum_{g'} \Sigma_{g'\to g}\phi_{g'} + S_g \tag{2-1-25}$$

$$\phi_g \equiv \int_{u_{g-1}}^{u_g} \phi(u)\,du \tag{2-1-26}$$

$$\Sigma_{t,g} \equiv \frac{\int_{u_{g-1}}^{u_g} \Sigma_t(u)\phi(u)\,du}{\phi_g} \tag{2-1-27}$$

$$\Sigma_{g'\to g} \equiv \frac{\int_{u_{g'-1}}^{u_{g'}} \phi(u')\int_{u_{g-1}}^{u_g} \Sigma(u'\to u)\,du\,du'}{\phi_g} \tag{2-1-28}$$

$$S_g \equiv \int_{u_{g-1}}^{u_g} S(u)\,du \quad . \tag{2-1-29}$$

The group number g increases as the lethargy increases (in other words, as the energy decreases). u_g is the lethargy value at the boundary between the gth and the $(g+1)^{th}$ energy groups, with the following:

$$u_0 = 0 \quad . \tag{2-1-30}$$

The value for $\phi(u)$ in Eqs. (2-1-26) through (2-1-28) has not yet been found, but it can be approximated mostly in good accuracy, allowing us to evaluate $\Sigma_{t,g}$ and $\Sigma_{g'\text{-}g}$, which can then be used in Eq. (2-1-25) to solve for ϕ_g. Equation (2-1-25) is called the *multigroup equation*. When G takes a small value, it is called the *few group approximation*. $\Sigma_{t,g}$ and $\Sigma_{g'\text{-}g}$ are called *group constants*.

When the change in cross section with neutron energy is small, there are no problems in solving the above equations. Generally, however, fissile and fertile nuclides have many sharp resonance peaks. The form of $\phi(u)$ is then strongly influenced by resonances in this cross section. Let us describe a typical approximation for $\phi(u)$ used when calculating the group constant in the resonance region. Here we need only a relative value for $\phi(u)$, rather than an absolute value. If the medium consists of an absorbent and a moderator, we obtain the following, which corresponds to Eq. (2-1-21):

$$[\Sigma_{at}(u) + \Sigma_{mt}]\phi(u) = \int_{u-\varepsilon_a}^{u} \Sigma_{as}(u')\phi(u')\frac{\exp(u'-u)\,du'}{1-\alpha_a}$$
$$+ \int_{u-\varepsilon_m}^{u} \Sigma_{ms}\phi(u')\frac{\exp(u'-u)}{1-\alpha_m}\,du' \quad . \tag{2-1-31}$$

Here, the subscripts a and m have been added to indicate the absorbent and the moderator, respectively. It is assumed here that the lethargy is quite large, so that there are no direct components from external sources. ε_m is also assumed to be much larger than the resonance width of the absorbent, so the second term on the right side of Eq. (2-1-31) can be approximated with a coefficient independent of u. In other words,

$$[\Sigma_{at}(u) + \Sigma_{mt}]\phi(u) = \int_{u-\varepsilon_a}^{u} \Sigma_{as}(u')\phi(u')\frac{\exp(u'\to u)}{1-\alpha_a}\,du' + S_m \quad . \tag{2-1-32}$$

Next, let us consider two extreme cases of the resonance width of the absorbent and ε_a. If ε_a is much greater than the resonance width, the first term on the right side of Eq. (2-1-32) can be approximated as a constant independent of u:

$$[\Sigma_{at}(u) + \Sigma_{mt}]\phi(u) = S_a + S_m \quad . \tag{2-1-33}$$

In other words,

$$\phi(u) = \frac{S_a + S_m}{\Sigma_{at}(u) + \Sigma_{mt}} \quad . \tag{2-1-34}$$

This is called the *narrow resonance approximation* (NR approximation). Next, let us consider the opposite case, where ε_a is considerably smaller than the resonance width. Then, $\Sigma_{as}(u)\phi(u)$ can be treated as a constant for $u - \varepsilon_a < u' < u$ in Eq.(2-1-32). Accordingly,

$$[\Sigma_{at}(u) + \Sigma_{mt}]\phi(u) = \Sigma_{as}(u)\phi(u) + S_m \quad . \tag{2-1-35}$$

In other words,

$$\phi(u) = \frac{S_m}{\Sigma_{aa}(u) + \Sigma_{mt}} \quad . \tag{2-1-36}$$

This is called the *wide resonance approximation* (WR approximation) or the *infinite mass approximation* (IM approximation).

Between the NR approximation and the WR approximation lies the *intermediate resonance approximation* (IR approximation), between Eq. (2-1-35) and Eq. (2-1-32) and can be approximated as:

$$[\Sigma_{at}(u) + \Sigma_{mt}]\phi(u) = (1 - \lambda)\Sigma_{as}(u)\phi(u) + \lambda S_a + S_m \quad . \tag{2-1-37}$$

In other words,

$$\phi(u) = \frac{\lambda S_a + S_m}{\Sigma_{aa}(u) + \lambda \Sigma_{as}(u) + \Sigma_{mt}} \quad . \tag{2-1-38}$$

Here, $\lambda = 1$ corresponds to the NR approximation and $\lambda = 0$ to the WR approximation. Generally, λ falls somewhere between the two. It is clear from Eqs. (2-1-34), (2-1-36), and (2-1-38), that $\phi(u)$ takes a small value at the resonance points. Because of this, around resonance, the reaction rate becomes smaller than the values obtained using a constant value for $\phi(u)$. This effect is called *self-shielding*.

(2-1-5) Neutron Diffusion

(2-1-5-1) Multigroup Transport Model

This section also addresses the steady state condition. It is impossible to solve the general, unmodified form of Eq. (2-1-6) with currently available calculation resources. However, if the multigroup approach described in Section (4-2) is employed, it can be solved with the finite-difference approximation for simple problems:

$$\Omega \cdot \nabla \phi_g(r,\Omega) + \Sigma_{t,g}(r)\phi_g(r,\Omega) = \sum_{g'} \int_{4\pi} d\Omega' \Sigma_{s,g' \to g}(r,\Omega' \cdot \Omega)\phi_{g'}(r,\Omega')$$

$$+ \frac{x_g}{4\pi} \sum_{g'} \nu\Sigma_{f,g'}(r)\phi_{g'}(r) + S_g(r,\Omega) \quad . \tag{2-1-39}$$

Here, a distinction has been made between nuclear fission and other neutron-emitting reactions. The difference between $\phi_g(r,\Omega)$ and $\phi_g(r)$ should be considered as mentioned in Section (2). If there is no external neutron source, a steady state exists only at a critical state. When the system is not at a critical state, the effective neutron multiplication factor can be introduced to handle this calculation. This is further explained in Section (5-2) for the multigroup diffusion model. The reader should be aware that the solution method explained below must be modified somewhat in Section (5-2).

Generally, an initial value is assumed for $\phi_g(r,\Omega)$ and iteration is performed in order to solve Eq. (2-1-39). Then, if the ith iteration of ϕ_g is written $\phi_g^{(i)}$, the following iteration formula is used:

$$\Omega \cdot \nabla \phi_g^{(i)}(r,\Omega) + \Sigma_{t,g}(r)\phi_g^{(i)}(r,\Omega) - \sum_{g'} \int_{4\pi} d\Omega \Sigma_{s,g' \to g}(r,\Omega \cdot \Omega)\phi_{g'}^{(i)}(r,\Omega)$$

$$= \frac{x_g}{4\pi} \sum_{g'} \nu\Sigma_{f,g'}(r)\phi_{g'}^{(i-1)}(r) + S_g(r,\Omega) \quad . \tag{2-1-40}$$

Here, $\phi_g^{(i-1)}$ in the first term of the right side are treated as $\phi_g^{(i)}$ to make the convergence faster. It is common to carry out repeated computations to solve Eq. (2-1-40). These iterations are often called *source iterations* or *outer iterations*. See Section (5-3) for further details.

There are two ways to handle $\Sigma_{s,g' \to g}(r,\Omega' \cdot \Omega)$ with the variable $\mu_0 = \Omega' \cdot \Omega$. One is by a Legendre function expansion, and the other by discretization of μ_0. If $\Sigma_{s,g' \to g}(r, \mu_0)$ is expanded with a Legendre function, Eq. (2-1-40) can be solved for $\phi_g^{(i)}(r,\Omega)$ by expanding a spherical harmonic series with finite terms. This is often called the P_N *method*. Alternatively, Ω can be discretized to find $\phi_g^{(i)}(r,\Omega)$. In this case, $\Sigma_{s,g' \to g}(r,\Omega' \cdot \Omega)$ can be expanded with a Legendre function or discretized with μ_0. This method is usually called the S_N *method*. Both the P_N and the S_N methods are handled by discretizing r. At present, the S_N method is much more commonly used.

(2-1-5-2) Multigroup Diffusion Model

Commonly, the quantity of interest is an integral value with the neutron flux as a weighting function, such as reaction rates. For this case, even if the neutron angular flux $\phi_g(r,\Omega)$ is unknown, it is sufficient to know the scalar neutron flux $\phi_g(r)$. When Eq. (2-1-39) is integrated over Ω, we

obtain the following expression:

$$\nabla \cdot J_g(r) + \Sigma_{t,g}(r)\phi_g(r) = \sum_{g'}\Sigma_{s,g'\to g}(r)\phi_{g'}(r) + x_g\sum_{g'}\nu\Sigma_{f,g'}(r)\phi_{g'}(r) + S_g(r) \quad , \qquad (2\text{-}1\text{-}43)$$

where $J_g(r)$ is a quantity known as the *neutron current*, defined as:

$$J_g(r) \equiv \int_{4\pi}\Omega\phi_g(r,\Omega)d\Omega \quad , \qquad (2\text{-}1\text{-}44)$$

and $\Sigma_{s,g'\to g}(r)$ is the following:

$$\Sigma_{s,g'\to g}(r) \equiv \int_{4\pi}\Sigma_{s,g'\to g}(r,\Omega'\cdot\Omega)d\Omega \quad . \qquad (2\text{-}1\text{-}45)$$

Once the relation between $J_g(r)$ and $\phi_g(r)$ is known, it can be combined with Eq. (2-1-43) to find $\phi_g(r)$. Expanding $\phi_g(r,\Omega)$ about Ω, we obtain:

$$\phi_g(r,\Omega) = \frac{1}{4\pi}[\phi_g(r) + 3\Omega \cdot J_g(r)] + \cdots \quad . \qquad (2\text{-}1\text{-}46)$$

If this is expanded only to the first term and substituted into Eq. (2-1-39), multiplied by Ω, and integrated over Ω, we obtain:

$$\frac{1}{3}\nabla\phi_g(r) + \Sigma_{t,g}(r)J_g(r) = \sum_{g'}\mu_0\Sigma_{s,g'\to g}(r)J_{g'}(r) + S'_g(r) \quad , \qquad (2\text{-}1\text{-}47)$$

where the following identities are used:

$$\mu_0 \equiv \frac{\int_{4\pi}\Omega'\cdot\Omega\Sigma_{s,g'\to g}(r,\Omega'\cdot\Omega)d\Omega}{\Sigma_{s,g'\to g}(r)} \qquad (2\text{-}1\text{-}48)$$

$$S'_g(r) \equiv \int_{4\pi}\Omega S_g(r,\Omega)d\Omega \quad . \qquad (2\text{-}1\text{-}49)$$

Table 2-1-2 Formula of Ω-integration

$$\int A d\Omega = 4\pi A$$
$$\int \Omega A d\Omega = 0$$
$$\int \Omega(\Omega \cdot A)\, d\Omega = \frac{4\pi}{3} A$$

The formula used for integrating over Ω is shown in Table 2-1-2. $S_g(r,\Omega)$ is generally isotropic; therefore,

$$S'_g(r) = 0 \quad . \tag{2-1-50}$$

Also, if the energy is fairly low, scattering is isentropic with respect to the center of mass system, resulting in:

$$\mu_0 = \frac{2}{3A} \quad . \tag{2-1-51}$$

Equation (2-1-47) resembles Fick's law for diffusion phenomena. In other words, if we neglect the terms relating to scattering to other exterior groups, we obtain:

$$J_g(r) = -D_g(r)\nabla\phi_g(r) \quad , \tag{2-1-52}$$

and Fick's law is satisfied. Here,

$$D_g(r) = \frac{1}{3[\Sigma_{t,g}(r) - \mu_0 \Sigma_{s,g' \to g}(r)]} \quad . \tag{2-1-53}$$

Substituting Eq. (2-1-52) into Eq. (2-1-43), we obtain:

$$-\nabla \cdot D_g(r)\nabla\phi_g(r) + \Sigma_{r,g}(r)\phi_g(r) = \sum_{g' \neq g}\Sigma_{s,g' \to g}(r)\phi_{g'}(r) + x_g\sum_{g'}\nu\Sigma_{f,g'}(r)\phi_{g'}(r) + S_g(r) \quad . \tag{2-1-54}$$

Here, the two self-scattering terms cancel each other. $\Sigma_{r,g}(r)$ is called the *removal cross-section* and is defined by the following:

$$\Sigma_{r,g}(r) \equiv \Sigma_{t,g}(r) - \Sigma_{s,g \to g}(r) \quad . \tag{2-1-55}$$

Also, the quantity:

$$\Sigma_{tr,g}(r) \equiv \Sigma_{t,g}(r) - \mu_0 \Sigma_{s,g \to g}(r) \tag{2-1-56}$$

is called the *transport cross-section*. In addition, the reciprocal of the transport cross-section is called the *transport mean-free-path* and is represented by λ_{tr}:

$$\lambda_{tr} \equiv \Sigma_{tr,g}(r)^{-1} \quad . \tag{2-1-57}$$

Using $\Sigma_{tr,g}(r)$, $D_g(r)$ can be written as follows, from Eq. (2-1-53):

$$D_g(r) = [3\Sigma_{tr,g}(r)]^{-1} \quad . \tag{2-1-58}$$

Table 2-1-3 shows the shape of $\nabla \cdot D\nabla$ in a representative coordinate system. In contrast to the *multigroup transport equation* of Eq. (2-1-39), Eq. (2-1-54) is called the *multigroup diffusion equation*.

Table 2-1-3　Forms for $\nabla \cdot D\nabla$

- rectangular (x, y, z)

$$\frac{\partial}{\partial x}D\frac{\partial}{\partial x}+\frac{\partial}{\partial y}D\frac{\partial}{\partial y}+\frac{\partial}{\partial z}D\frac{\partial}{\partial z}$$

- cylindrical (r, ϕ, z)

$$\frac{1}{r}\frac{\partial}{\partial r}rD\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial}{\partial \phi}D\frac{\partial}{\partial \phi}+\frac{\partial}{\partial z}D\frac{\partial}{\partial z}$$

- spherical (r, θ, ϕ)

$$\frac{1}{r^2}\frac{\partial}{\partial r}r^2D\frac{\partial}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\sin\theta D\frac{\partial}{\partial \theta}+\frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial \phi}D\frac{\partial}{\partial \phi}$$

Since the transport equation faithfully represents the transport of neutrons, the *boundary conditions* are clearly defined. When the system has a *vacuum boundary*, the neutron flux into the system from outside can be considered to be zero. In contrast, since the diffusion equation is an approximate equation, its boundary conditions are not always self-evident. A sufficient approximation is to require continuity of $\phi_g(r)$ and $J_g(r)$ at the boundary between two adjacent regions. Another boundary condition is the symmetric condition that the gradient of the neutron flux must be zero along the centerlines. An additional condition is generally imposed at a vacuum boundary: $\phi_g(r)$ must reach zero at a distance d in the vacuum from the massive region outer boundary, called the *extrapolation distance*. This is generally written:

$$\phi(R+d)=0 \qquad . \tag{2-1-59}$$

It can also be written:

$$\frac{d\phi}{dn}=-\frac{\phi}{d} \qquad . \tag{2-1-60}$$

The extrapolation distance can also be formulated as follows, taking advantage of transport theory:

$$d=0.7104\lambda_{tr} \qquad . \tag{2-1-61}$$

Here, λ_{tr} is the transport mean-free-path, as defined in Eq. (2-1-57).

While the transport equation is used for calculations regarding shielding, control rods, and other components of a nuclear reactor, the diffusion equation is mainly used for the entire reactor core. Fuel elements are arrayed in the core, in a regular but complicated pattern. Because of this, calculations of the group constant must account not only for cross section change with neutron energy, but also for the effects of fine geometric structure. The calculations are carried out for a fuel cell, such as individual fuel elements and a fuel assembly, and are called *cell calculations*. The transport equation is solved in cell calculations; usually, the *collision probability method* is employed, which solves the transport equation in an integrative form, by dividing the unit cell

into multiple small regions.

(2-1-5-3) Iterative Calculations for Neutron Sources

This section describes source iteration, as mentioned in Section (5-1). As already explained, this is also sometimes called *outer iteration*, but this term is used for several different techniques, so the reader should take care as to which technique is being referred to. The transport equation is given in Eq. (2-1-40), but can be revised to resemble the diffusion equation (2-1-54):

$$-\nabla \cdot D_g(r)\nabla \phi_g^{(i)}(r) + \Sigma_{r,g}(r)\phi_g^{(i)}(r) - \sum_{g'\neq g}\Sigma_{s,g'\to g}(r)\phi_{g'}^{(i)}(r) = x_g\sum_{g'}v\Sigma_{f,g'}(r)\phi_{g'}^{(i-1)}(r) + S(r) \quad .$$

$$(2\text{-}1\text{-}62)$$

The diffusion equation will be described here, but the same considerations can be applied to the transport equation.

Different iterative calculation methods are used for different treatment of $S(r)$, with $S(r)$ being defined by the problem. The problem is to obtain the shape of the neutron flux for a given $S(r)$. The usual procedure is to solve Eq. (2-1-62), including $S(r)$. However, another method of solving the equation is presented here, in which $S(r)$ is incorporated in the initial calculation but subtracted from the later iterative calculation:

$$-\nabla \cdot D_g(r)\nabla \phi_g^{(0)}(r) + \Sigma_{r,g}(r)\phi_g^{(0)}(r) - \sum_{g'\neq g}\Sigma_{s,g'\to g}(r)\phi_{g'}^{(0)}(r) = S(r) \qquad (2\text{-}1\text{-}63)$$

$$-\nabla \cdot D_g(r)\nabla \phi_g^{(i)}(r) + \Sigma_{r,g}(r)\phi_g^{(i)}(r) - \sum_{g'\neq g}\Sigma_{s,g'\to g}(r)\phi_{g'}^{(i)}(r) = x_g\sum_{g'}v\Sigma_{f,g'}(r)\phi_{g'}^{(i-1)}(r)$$

$$\text{for} \qquad i \geq 1 \qquad (2\text{-}1\text{-}64)$$

Here, $\phi_g^{(0)}$ describes the distribution of the neutron flux created by the neutrons emitted by the source, but that have not yet caused any fissions. The neutrons released due to fissions caused by $\phi_g^{(0)}$ are represented by $\phi_g^{(1)}$. Accordingly, the neutrons in flux $\phi_g^{(i)}$ are those emitted due to fissions caused by $\phi_g^{(i-1)}$. As the value of i in $\phi_g^{(i)}$ increases, ϕ_g converges to zero in a non-critical system. The actual solution, i.e., the physically manifested neutron flux, is given by:

$$\phi_g(r) = \sum_{i=0}^{\infty}\phi_g^{(i)}(r) \quad . \qquad (2\text{-}1\text{-}65)$$

The term $\phi_g^{(i)}$ takes on different physical meanings between Eq. (2-1-62) and the set of Eqs. (2-1-63) and (2-1-64), so the reader should take care not to confuse these terms. The answer for Eq. (2-1-62) is:

$$\phi_g(r) = \phi_g^{(\infty)}(r) \quad . \qquad (2\text{-}1\text{-}66)$$

This method is often called power method. We will discuss about it in Sec. (2-2-2-1).

We can solve this problem by the iteration given by Eq. (2-1-62). A set of initial guess values is assumed for $\phi_g^{(0)}$ and then corrected using Eq. (2-1-62), to approach the correct solution. Equation (2-1-62) is useful when trying to find the most accurate possible approximation, but otherwise, it is better to use Eqs. (2-1-63) and (2-1-64), since the physical meaning of these is clear.

When analyzing a nuclear reactor core, we are almost always analyzing a core in the critical condition. In this case, there are no external neutron sources, so Eq. (2-1-54) can be re-written as:

$$-\nabla \cdot D_g(r)\nabla\phi_g(r) + \Sigma_{r,g}(r)\phi_g(r) - \sum_{g'\neq g}\Sigma_{s,g'\rightarrow g}(r)\phi_{g'}(r) = x_g\sum_{g'}\nu\Sigma_{f,g'}(r)\phi_{g'}(r) \quad .$$

(2-1-67)

This expression sets no absolute value for $\phi_g(r)$, which instead is set by the selection of the power output. The coefficients of Eq. (2-1-67) must be chosen so the equation is exactly satisfied, namely the system is just in critical state, which is difficult to do. Ordinarily, an *effective multiplication factor* k_{eff} is introduced for avoiding this problem. The equation then changes as shown here:

$$-\nabla \cdot D_g(r)\nabla\phi_g(r) + \Sigma_{r,g}(r)\phi_g(r) - \sum_{g'\neq g}\Sigma_{s,g'\rightarrow g}(r)\phi_{g'}(r) = \frac{x_g}{k_{eff}}\sum_{g'}\nu\Sigma_{f,g'}(r)\phi_{g'}(r) \quad .$$

(2-1-68)

This is usually solved by performing the following iteration:

$$-\nabla \cdot D_g(r)\nabla\phi_g^{\left(i-\frac{1}{2}\right)}(r) + \Sigma_{r,g}(r)\phi_g^{\left(i-\frac{1}{2}\right)}(r) - \sum_{g'\neq g}\Sigma_{s,g'\rightarrow g}(r)\phi_{g'}^{\left(i-\frac{1}{2}\right)}(r) = x_g\sum_{g'}\nu\Sigma_{f,g'}(r)\phi_{g'}^{(i-1)}(r) \quad .$$

(2-1-69)

Here k_{eff} is obtained from:

$$k_{eff}^{(i)} = \frac{\int\sum_{g'}\Sigma_{f,g'}(r)\phi_{g'}^{\left(i-\frac{1}{2}\right)}(r)dr}{\int\sum_{g'}\Sigma_{f,g'}(r)\phi_{g'}^{(i-1)}(r)dr} \quad .$$

(2-1-70)

If $\phi_g^{(i)}$ is set as $\phi_g^{(i-\frac{1}{2})}$, in analogy to the iterative calculation using Eqs. (2-1-61) and (2-1-62). Eq. (2-1-69) resembles the change of neutron flux between generations, starting from the source given by:

$$S(r) = x_g\sum_{g'}\nu\Sigma_{f,g'}(r)\phi_{g'}^{(0)}(r) \quad .$$

Here, "generation" means those neutrons born in the preceding set of fissions that are absorbed or leaked by the time of the subsequent set of fissions. $k_{eff}^{(i)}$ represents the ratio of the number of fission reactions between the ith and $(i-1)^{th}$ generations, thus showing whether the number of neutrons increases.

Generally, in solving a criticality problem, it is not possible to match the calculation conditions exactly with the criticality conditions. This is problematic because the absolute value of the neutron flux will vary depending on the value of $k_{eff}^{(i)}$. To resolve this, the neutron flux is normalized as:

$$\int \sum_{g'} \Sigma_{f,g'}(r)\phi_{g'}^{(i)}(r)dr = P \qquad , \qquad (2\text{-}1\text{-}71)$$

where P is the total number of nuclear fissions, a constant determined by the power output. From Eqs. (2-1-70) and (2-1-71), we obtain the relation:

$$\int \sum_{g'} \Sigma_{f,g'}(r)\phi_{g'}^{\left(i-\frac{1}{2}\right)}(r)dr = k_{eff}^{(i)} P \quad .$$

The following equation can then be applied:

$$\phi_g^{(i)}(r) = \frac{1}{k_{eff}^{(i)}} \phi_g^{\left(i-\frac{1}{2}\right)}(r) \quad , \qquad (2\text{-}1\text{-}72)$$

which results in a neutron flux satisfying Eq. (2-1-71).

Let us summarize the above iterative calculations:

① An initial value of the neutron flux $\phi_g^{(0)}$ satisfying $\int \sum_{g'} \Sigma_{f,g'}(r)\phi_{g'}^{(0)}(r)dr = P$ is selected.

② Iterations are performed with the following expression from $i = 1$ until the value converges:

$$-\nabla \cdot D_g(r)\nabla\phi_g^{\left(i-\frac{1}{2}\right)}(r) + \Sigma_{r,g}(r)\phi_g^{\left(i-\frac{1}{2}\right)}(r) - \sum_{g'\neq g}\Sigma_{s,g'\to g}(r)\phi_{g'}^{\left(i-\frac{1}{2}\right)}(r) = x_g \sum_{g'} \nu\Sigma_{f,g'}(r)\phi_{g'}^{(i-1)}(r)$$

$$(2\text{-}1\text{-}69)$$

$$k_{eff}^{(i)} = \frac{\int \sum_{g'} \Sigma_{f,g'}(r)\phi_{g'}^{\left(i-\frac{1}{2}\right)}(r)dr}{P}$$

$$\phi_g^{(i)}(r) = \frac{1}{k_{eff}^{(i)}} \phi_g^{\left(i-\frac{1}{2}\right)}(r) \quad . \qquad (2\text{-}1\text{-}72)$$

Convergence is evaluated by $k_{eff}^{(i)}$ and the norms of $\phi_g^{(i)}(r)$.

As stated earlier, this is called an outer iteration. Sometimes, however, a further outer iteration is employed, adjusting the nuclide number density or other parameters in order to drive k_{eff} to 1. This is called a *criticality search calculation*.

Let us consider a little further the scattering term in Eq. (2-1-69), that is, the third term on the left side. A fraction of the thermal neutrons collide with nuclei and gain kinetic energy from the thermal motion energy of the nuclei. However, any kinetic energy greater than the thermal cutoff energy is lost due to neutron scattering. Because of this effect, in such energy groups, $\Sigma_{s,g\to g'}^{(r)}$ in which $g' > g$, becomes zero. If the fission term is non-zero, Eq. (2-1-69) can be solved successively from $g = 1$ to higher energy groups. For thermal neutron groups the same kind of iteration as the outer iteration is performed, although no such calculation is necessary for normalization with k_{eff}. These calculations allow the thermal neutron groups to be collapsed to a single group, thus simplifying the solution. This group is called a *thermal group*.

(2-1-5-4) 2-Group Diffusion Model

The neutron energy groups other than the thermal group can be treated as a single group, called the *fast group*. These are often handled in 2-group diffusion equations. For these calculations, Eq. (2-1-68) is re-written:

$$-\nabla \cdot D_1(r)\nabla \phi_1(r) + \Sigma_{r,1}(r)\phi_1(r) = \frac{f(r)\eta_T(r)\varepsilon(r)}{k_{eff}}\Sigma_{r,2}(r)\phi_2(r) \qquad (2\text{-}1\text{-}73)$$

$$-\nabla \cdot D_2(r)\nabla \phi_2(r) + \Sigma_{r,2}(r)\phi_2(r) = p(r)\Sigma_{r,1}(r)\phi_1(r) \quad . \qquad (2\text{-}1\text{-}74)$$

Here, $f(r)$, $\eta_T(r)$, $\varepsilon(r)$, and $p(r)$ are parameters described by a four-factor formula. Equation (2-1-73) can also be written as:

$$-\nabla \cdot D_1(r)\nabla \phi_1(r) + \Sigma_{r,1}(r)\phi_1(r) = \frac{k_\infty(r)}{k_{eff}}\frac{\Sigma_{r,2}(r)}{p(r)}\phi_2(r) \quad . \qquad (2\text{-}1\text{-}75)$$

Here, $k_\infty(r)$ is the neutron multiplication factor for an infinite medium described in the previous section.

The value of D_1 divided by $\Sigma_{r,1}$:

$$\tau = \frac{D_1}{\Sigma_{r,1}} \qquad (2\text{-}1\text{-}76)$$

is called the *Fermi age* or simply *age*. If the neutron energy is treated as a continuous quantity, it can be calculated thus:

$$\tau = \int_0^{u_T} \frac{D(u)}{\xi \Sigma_s(u)} du \quad . \qquad (2\text{-}1\text{-}77)$$

Here, u_T is the lethargy corresponding to thermal neutrons. For a neutron emitted from a point source with a lethargy of zero and then repeatedly slowed down or scattered, τ can also be written as:

$$\tau = \frac{1}{6} < r_1^2 > , \qquad (2\text{-}1\text{-}78)$$

where $<r_1^2>$ is the mean square of the distance from the point neutron source to the position at which the lethargy passes u_T during slow down. This value can be measured using a point source of fast neutrons and a thermal neutron counter. Values of τ are shown in Table 2-1-4 for typical moderators with some other diffusion parameters. In this table τ is given also for typical thermal reactors. It is known that the core volume is proportional to $\tau^{3/2}$ for typical thermal reactors.[2]

The square root of D_2 divided by $\Sigma_{r,2}$:

$$L = \left(\frac{D_2}{\Sigma_{r,2}}\right)^{1/2} \qquad (2\text{-}1\text{-}79)$$

is called the *diffusion length* of thermal neutrons. L^2 can be stated in terms of the mean square

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$\langle r_2{}^2\rangle$ of the distance traveled by thermal neutrons from the source to the absorption site:

$$L^2 = \frac{1}{6} < r_2{}^2 > \quad .$$

(2-1-80)

Like τ, this quantity can be measured using a thermal neutron source and a thermal neutron detector, but it is difficult to obtain a point source of neutrons. Exponential experiments and/or pulse experiments are performed instead.

Table 2-1-4   Diffusion parameters for some common moderators[1]

Moderator (reactor type)	Density g/cm^3	D cm	Σa cm^{-1}	L cm	τ cm^2	M cm
H₂O	1.00	0.16	2.0E-02	2.85	26	5.84
D₂O	1.10	0.87	2.9E-05	170	131	170
Be	1.85	0.50	1.0E-03	21	102	23
Graphite	1.60	0.84	2.4E-04	59	368	62
PWR				1.8	40	6.6
BWR				2.2	50	7.3
HTGR				12.0	300	21

Let us consider a simple case in which the coefficients in Eqs. (2-1-74) and (2-1-75) do not depend on r. Those expressions can then be written as follows:

$$-\tau \nabla^2 \phi_1(r) + \phi_1(r) = \frac{k_\infty}{k_{eff}} \frac{\Sigma_{r,2}}{p\,\Sigma_{r,1}} \phi_2(r)$$

(2-1-81)

$$-L^2 \nabla^2 \phi_2(r) + \phi_2(r) = \frac{p\Sigma_{r,1}}{\Sigma_{r,2}} \phi_1(r) \quad .$$

(2-1-82)

It is clear that these solutions satisfy the following expression:

$$\nabla^2 \phi_g(r) + B_G^2 \phi_g(r) = 0 \quad .$$

(2-1-83)

Here, B_G^2 is a quantity called *geometrical buckling*, an eigenvalue determined by satisfying certain boundary conditions. Let us assume that the differences in Eq. (2-1-83) between Group 1 and Group 2 can be neglected, so that B_G^2 is the same in both groups. Table 2-1-5 shows the geometrical buckling that occurs in typical core shapes and the corresponding neutron flux distribution.

Table 2-1-5 Geometrical buckling and flux profile

geometry	geometrical buckling	flux profile
slab thickness, H	$\left(\dfrac{\pi}{H}\right)^2$	$\cos\left(\dfrac{\pi x}{H}\right)$
infinite cylinder radius, R	$\left(\dfrac{2.405}{R}\right)^2$	$J_0\left(\dfrac{2.405\ r}{R}\right)$
sphere radius, R	$\left(\dfrac{\pi}{R}\right)^2$	$\dfrac{1}{r}\cos\left(\dfrac{\pi r}{R}\right)$
rectangular side lengths, A, B, C	$\left(\dfrac{\pi}{A}\right)^2+\left(\dfrac{\pi}{B}\right)^2+\left(\dfrac{\pi}{C}\right)^2$	$\cos\left(\dfrac{\pi x}{A}\right)\cos\left(\dfrac{\pi y}{B}\right)\cos\left(\dfrac{\pi z}{C}\right)$
finite cylinder radius, R; height, H	$\left(\dfrac{2.405}{R}\right)^2+\left(\dfrac{\pi}{H}\right)^2$	$J_0\left(\dfrac{2.405\ r}{R}\right)\cos\left(\dfrac{\pi x}{H}\right)$

J_0 is the zero-th order Bessel function.

Substituting Eq. (2-1-83) into Eqs. (2-1-81) and (2-1-82), we obtain:

$$(\tau B_G^2 + 1)\phi_1(r) = \frac{k_\infty}{k_{eff}}\frac{\Sigma_{r,2}}{p\Sigma_{r,1}}\phi_2(r) \qquad (2\text{-}1\text{-}84)$$

$$(L^2 B_G^2 + 1)\phi_2(r) = \frac{p\Sigma_{r,1}}{\Sigma_{r,2}}\phi_1(r) \quad . \qquad (2\text{-}1\text{-}85)$$

Since both expressions must be satisfied simultaneously, the following must be satisfied:

$$(1 + \tau B_G^2)(1 + L^2 B_G^2) = \frac{k_\infty}{k_{eff}} \quad . \qquad (2\text{-}1\text{-}86)$$

In examining this equation, it is clear that τB_G^2 represents the fraction of fast neutrons leaking from the system and $L^2 B_G^2$ represents the fraction of thermal neutrons leaking from a thermal system. The fractions are generally small, and thus Eq. (2-1-86) changes form as follows:

$$k_{eff} = \frac{k_\infty}{1 + M^2 B_G^2} \quad . \qquad (2\text{-}1\text{-}87)$$

Here, M^2 is called the *migration area* and is defined by:

$$M^2 = \tau + L^2 \qquad . \qquad (2\text{-}1\text{-}88)$$

At criticality, $k_{eff} = 1$, so from Eq. (2-1-87),

$$\frac{k_\infty}{1 + M^2 B_G^2} = 1 \quad . \tag{2-1-89}$$

Under non-critical conditions, from

$$\frac{k_\infty}{1 + M^2 B_M^2} = 1 \quad , \tag{2-1-90}$$

we define the *material buckling* as:

$$B_M^2 = \frac{k_\infty - 1}{M^2} \quad . \tag{2-1-91}$$

Then, the critical condition can be rewritten as:

$$B_M^2 = B_G^2 \quad . \tag{2-1-92}$$

At sub-critical conditions, k_{eff} is introduced to obtain non-zero solutions. In sub-critical systems containing neutron sources, $k_{eff} = 1$ must be substituted in Eqs. (2-1-81) and (2-1-82). We assume that the relative spatial distributions of $\phi_1(r)$ and $\phi_2(r)$ are identical and make the same transformations as previously used in this chapter, obtaining:

$$\nabla^2 \phi_g(r) + B_M^2 \phi_g(r) = 0 \tag{2-1-93}$$

for any time and position, where the external neutron source does not exist. In this case, there is an external neutron source sustaining the neutron flux and the reader should be aware that the conditions here differ from criticality. It should be clear from this equation that material buckling can be measured in exponential experiments and pulse experiments. Here reactor physics experiments are out of scope, and their discussion are omitted.

References

1) J. J. Duderstadt and L. J. Hamilton, "Nuclear Reactor Analysis," John Wiley and Sons, Inc., New York (1976).

2) H. Sekimoto, Genshiryoku-kogyo, **27[4]**, 81(1981) (in Japanese).

Part 2-2
Numerical Analysis of Diffusion Equation

(2-2-1) Discretization of Diffusion Equation

We start the numerical analysis of diffusion equation with discretization of multigroup diffusion equation, which is given by Eq. (2-1-54) for an external source problem and Eq. (2-1-68) for a criticality problem. The derived equation from diffusion equation is called *difference equation*. The space is discretized into small enough elements. This element is called *mesh*. A value of neutron flux is chosen for each mesh. This procedure makes a continuous function of space variable into a set of discrete values. The balance of neutron flux expressed originally by integro-differential equation is changed into a difference equation, which is equivalent to a matrix equation. The matrix equation is usually much easier to be treated by computer than the function equation. This is a principle of discretization method.

Boundaries of regions should usually be chosen of the boundaries of meshes. The most popular discretization method for multidimensional case is to discretize each coordinate and construct each space mesh surrounded by these discretized coordinates. The value of neutron flux for each mesh may be chosen by several methods, but here we choose the value at the center of mesh. The definition of center is not so rigid, since we are treating it approximately. We may often consider this value as some average value in this mesh.

The derivation of the difference equation from the diffusion equation is straight forward and relatively easy except for the diffusion term, which is a second order differential term. Here we mostly discuss the treatment of the diffusion term. The other terms are products of neutron fluxes and their corresponding coefficients. They should be transformed to the product of an averaged neutron flux in each mesh and a proper coefficient, which is estimated to give the value of integrated product in the mesh. If the cell is one material, the process is easy. However, in many cases, the mesh consists of many components such as fuel pellet, cladding, coolant and others, and calculating coefficients becomes a complicated procedure. In this case the mesh is often called *cell*. This process is called cell calculation. We have omitted this part from this textbook.

Next, we describe the treatment of the diffusion term. We shall not consider the energy variable in the mean time, and omit the suffix of the energy group in the equations. The diffusion term of the one-dimensional diffusion equation is written as:

$$-\nabla \cdot D\nabla \phi = -\frac{1}{r^p}\left[\frac{d}{dr}\left(r^p D \frac{d\phi}{dr}\right)\right], \tag{2-2-1}$$

where p is chosen for the corresponding geometry as follows:

$$p = \begin{cases} 0: & \text{plane} \\ 1: & \text{cylinder} \\ 2: & \text{sphere} \end{cases}.$$

Even for a multidimensional case, the diffusion term can be expressed by combining the terms given by Eq. (2-2-1), since angular coordinates are seldom used.

In the following, the discretization of Eq. (2-2-1) is described. Usually two methods can be considered. One is the direct mathematical derivation of the difference equation from the differential equation, and the other is the physical derivation by considering the material balance in the mesh. Generally the latter method gives a more accurate expression of coefficients. Here we will employ the latter method and derive the difference equation for Eq. (2-2-1). We will not consider the original diffusion equation directly, but the equation multiplied by r^p. We assume in

each mesh a proper value is given for each parameter such as a macroscopic cross-section and a diffusion coefficient. Each boundary of the region should be chosen as a boundary of mesh.

At the beginning each space coordinate r is divided into K meshes. We will consider the neutron balance in the k-th mesh, which is called k-mesh. The left and right edges of the mesh are denoted by $r_{k-1/2}$ and $r_{k+1/2}$, respectively, and the mesh width is denoted by Δr_k. The diffusion term represents the balance between coming-in neutron current at $r = r_{k-1/2}$ and going-out current at $r = r_{k+1/2}$, namely:

$$-\nabla \cdot D \nabla \phi \mid_k = \left(r^p J \mid_{k+1/2} - r^p J \mid_{k-1/2} \right) \times \frac{p+1}{r_{k+1/2}^{p+1} - r_{k-1/2}^{p+1}}, \tag{2-2-2}$$

where the second term in the right hand side is the reciprocal of mesh volume.

The neutron current at $r = r_{k-1/2}$ is estimated by using the diffusion approximation as:

$$J_{k-1/2} = -D \frac{d\phi}{dr} \mid_{k-1/2}. \tag{2-2-3}$$

Now we try to change differential to difference. Several methods may be considered for this discretization. Here we consider the neutron current from $(k-1)$-mesh to this boundary. It can be estimated as:

$$J_{k-1/2-} = -D_{k-1} \frac{\phi_{k-1/2} - \phi_{k-1}}{\Delta r_{k-1}/2}. \tag{2-2-4}$$

By using the same method, the current to $(k+1)$-mesh from this boundary can be estimated as:

$$J_{k-1/2+} = -D_k \frac{\phi_k - \phi_{k-1/2}}{\Delta r_k/2}. \tag{2-2-5}$$

From the continuity of the neutron current, these two quantities are equal and considered the current at this point, $J_{k-1/2}$:

$$J_{k-1/2-} = J_{k-1/2+} = J_{k-1/2}. \tag{2-2-6}$$

By eliminating $\phi_{k-1/2}$ from Eqs. (2-2-4) through (2-2-6) the following equation is given for $J_{k-1/2}$:

$$J_{k-1/2} = -2 \left(\frac{\Delta r_{k-1}}{D_{k-1}} + \frac{\Delta r_k}{D_k} \right)^{-1} (\phi_k - \phi_{k-1}). \tag{2-2-7}$$

The equation for $J_{k+1/2}$ is also given by the similar way as:

$$J_{k+1/2} = -2 \left(\frac{\Delta r_k}{D_k} + \frac{\Delta r_{k+1}}{D_{k+1}} \right)^{-1} (\phi_{k+1} - \phi_k). \tag{2-2-8}$$

By substituting (2-2-7) and (2-2-8) into Eqs. (2-2-2):

$$-\nabla \cdot D \nabla \phi \,|_k = -2 \left[r_{k+1/2}^{p} \left(\frac{\Delta r_k}{D_k} + \frac{\Delta r_{k+1}}{D_{k+1}} \right)^{-1} (\phi_{k+1} - \phi_k) - r_{k-1/2}^{p} \left(\frac{\Delta r_{k-1}}{D_{k-1}} + \frac{\Delta r_k}{D_k} \right)^{-1} (\phi_k - \phi_{k-1}) \right]$$

$$\times \frac{p+1}{r_{k+1/2}^{p+1} - r_{k-1/2}^{p+1}}$$

$$= c_{k-1} \phi_{k-1} + d'_k \, \phi_k + e_k \phi_{k+1} \tag{2-2-9}$$

where

$$c_{k-1} = -\frac{2(p+1) r_{k-1/2}^{p}}{\left(r_{k+1/2}^{p+1} - r_{k-1/2}^{p+1} \right) \left(\frac{\Delta r_{k-1}}{D_{k-1}} + \frac{\Delta r_k}{D_k} \right)} \tag{2-2-10}$$

$$e_k = -\frac{2(p+1) r_{k+1/2}^{p}}{\left(r_{k+1/2}^{p+1} - r_{k-1/2}^{p+1} \right) \left(\frac{\Delta r_k}{D_k} + \frac{\Delta r_{k+1}}{D_{k+1}} \right)} \tag{2-2-11}$$

$$d'_k = -c_{k-1} - e_k \quad . \tag{2-2-12}$$

We will now consider the boundary conditions. For cylindrical and spherical coordinate systems, the neutron current should be zero at the center. This condition is automatically satisfied by Eq. (2-2-10) as:

$$c_0 = 0 . \tag{2-2-13}$$

Hence, ϕ_0, which is the value at imaginary position, disappears in Eq. (2-2-9). An additional equation is not necessary for the boundary condition at the center.

Here we should note that the suffix at the central position is not 0 but 1/2. We choose an integer for each mesh, and half integer at each boundary. The mesh adjacent to the center usually takes the mesh number of 1. This numbering system is convenient when the whole system of equation is expressed by the matrix system.

The vacuum boundary condition is given by Eq. (2-1-59) by using the extrapolation distance d. This condition can be employed in the system of equations (2-2-9) by modifying the equation for e_K as:

$$e_K = -\frac{2(p+1) r_{K+1/2}^{p}}{\left(r_{K+1/2}^{p+1} - r_{K-1/2}^{p+1} \right) \left(\frac{\Delta r_K}{D_K} + \frac{2d}{D_K} \right)} = -\frac{2(p+1) r_{K+1/2}^{p}}{\left(r_{K+1/2}^{p+1} - r_{K-1/2}^{p+1} \right) \left(\frac{\Delta r_K}{D_K} + 4.262 \right)} \quad . \tag{2-2-14}$$

$-\nabla \cdot D \nabla \phi \,|_K$ is given by:

$$-\nabla \cdot D\nabla \phi \big|_K = c_{K-1}\phi_{K-1} + d'_K \phi_K \quad . \tag{2-2-15}$$

Next we may have to mention about 2- and 3- dimensional space, but rush to expression of difference equation form of multi-group neutron diffusion equation in matrix form, and will later mention about higher dimensional cases.

The neutron flux in space mesh k and energy group g is denoted by $\phi_{k,g}$, and the whole neutron flux is denoted by vector ϕ. The order of $\phi_{k,g}$ in ϕ is as follows:

$$\phi_{1,1},\ \phi_{2,1},\ \ldots,\ \phi_{K,1},\ \phi_{1,2},\ \phi_{1,2},\ \ldots,\ \phi_{1,2},\ \ldots,\ \phi_{1,g},\ \phi_{2,g},\ \ldots,\ \phi_{K,g},\ldots,\ \phi_{1,G},\ \phi_{2,G},\ \ldots,\ \phi_{K,G}.$$

Here the k changes first. The suffixes K and G are total space mesh number and total energy group number, respectively. This method changes the multi-group diffusion equation (2-2-68) as the following matrix equation:

$$T\phi = \frac{1}{k_{eff}} M\phi \quad , \tag{2-2-16}$$

where T and M are matrixes, whose structures are given in the following.

The matrix T is separated into two matrixes A and S as:

$$T = A - S \quad , \tag{2-2-17}$$

where matrix A correspond to the first and second terms of Eq. (2-2-68) and matrix S to the third term of the same equation. They are given by the following equations using element matrixes A_g and $S_{g',g}$:

$$A = \begin{bmatrix} A_1 & & & & & & \\ & A_2 & & & & 0 & \\ & & \cdot & & & & \\ & & & \cdot & & & \\ & & & & A_g & & \\ & & & & & \cdot & \\ & 0 & & & & & \cdot & \\ & & & & & & & A_G \end{bmatrix} \quad , \tag{2-2-18}$$

$$S = \begin{bmatrix} 0 & & & & & & \\ S_{1,2} & 0 & & & & 0 & \\ \cdot & & \cdot & & & & \\ \cdot & & & \cdot & & & \\ S_{1,g} & S_{2,g} & \cdot\cdot & S_{g-1,g} & 0 & & \\ \cdot & & & & \cdot & & \\ \cdot & & & & & \cdot & \\ S_{1,G} & S_{2,G} & \cdot\cdot & & \cdot\cdot & S_{G-1,G} & 0 \end{bmatrix} ,$$

(2-2-19)

where we assume up-scattering does not happen. If the thermal energy region consists of several energy groups, up-scattering should be considered. For this kind of case, some elements in the upper right of S will take some values other than zero. The element matrix A_g is a tri-diagonal matrix and given by:

$$A_g = \begin{bmatrix} d_1 & e_1 & & & & & \\ c_1 & d_2 & e_2 & & & 0 & \\ & \cdot & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & c_{k-1} & d_k & e_k & \\ & & & & \cdot & \cdot & \cdot \\ & 0 & & & & \cdot & \cdot & \cdot \\ & & & & & & c_{K-1} & d_K \end{bmatrix} ,$$

(2-2-20)

where the suffix g is omitted in every element of this matrix. The elements c_k and e_k are given by Eqs. (2-2-10) and (2-2-11), and d_k is given by:

$$d_k = d'_k + \Sigma_{r,k,g}$$

(2-2-21)

using d'_k given by Eq. (2-2-12), where $\Sigma_{r,k,g}$ is the removal cross section in the space mesh k and energy group g. The element matrix $S_{g',g}$ is a diagonal matrix whose size is K. The element of this matrix is the scattering matrix $\Sigma_{s,k,g'\to g}$ from energy group g' to g in space mesh k. For definition of each cross section, see Eq. (2-1-68).

The matrix M in Eq. (2-2-16) corresponds to the fission term and can be expressed as a product of two matrixes as:

$$M = XF^T ,$$

(2-2-22)

where matrixes X and F are column matrixes whose element matrixes are given as:

$$X = \left(X_1, \cdot\cdot, X_g, \cdot\cdot, X_G\right)^T ,$$

(2-2-23)

$$F = \left(F_1, \cdots, F_g, \cdots, F_G \right)^T \quad , \tag{2-2-24}$$

where matrixes X_g and F_g are square matrixes, whose sizes are K, and diagonal matrixes. The fission neutron spectrum χ_g can be assumed independent from the induced neutron energy and target nucleus and X_g can be written as:

$$X_g = \chi_g E \quad , \tag{2-2-25}$$

where E is a unit matrix. The k-th element of F_g is $\nu \Sigma_{f,k,g}$.

For a one-dimensional case, the matrix A_g becomes a tri-diagonal matrix. Here, the form of matrix A_g for multi-dimensional cases is explained. In the reactor analysis, almost all coordinate systems are rectangular, cylindrical or spherical (See Fig. 2-1-1, Table 2-1-3), and any other coordinate systems are rarely taken. Furthermore the ϕ-variable in cylindrical coordinates and ϕ- and θ-variable in spherical coordinates (Table 2-1-3) are rarely employed. Here we consider only (x, y, z) and (r, z) type coordinate systems.

For these coordinate systems, we start discretization process by discretizing each coordinate and setting mesh defined by the set of discretized coordinates. The neutron flux for 2- or 3-dimensional geometry is written as $\phi_{k,l}$ or $\phi_{k,l,m}$. In the same way as the one-dimensional case, $-\nabla \cdot D \nabla \phi \big|_{k,l}$ and $-\nabla \cdot D \nabla \phi \big|_{k,l,m}$ are expressed by using the adjacent fluxes. For a two-dimensional case:

$$-\nabla \cdot D \nabla \phi \big|_{k,l} = a'_{k,l;k,l} \phi_{k,l} + a_{k,l;k,l-1} \phi_{k,l-1} + a_{k,l;k,l+1} \phi_{k,l+1} + a_{k,l;k-1,l} \phi_{k-1,l} + a_{k,l;k+1,l} \phi_{k+1,l} \quad . \tag{2-2-26}$$

and for three-dimensional case:

$$\begin{aligned}
-\nabla \cdot D \nabla \phi \big|_{k,l,m} &= a'_{k,l,m;k,l,m} \phi_{k,l,m} + a_{k,l,m;k,l,m-1} \phi_{k,l,m-1} + a_{k,l,m;k,l,m+1} \phi_{k,l,m+1} \\
&+ a_{k,l,m;k,l-1,m} \phi_{k,l-1,m} + a_{k,l,m;k,l+1,m} \phi_{k,l+1,m} + a_{k,l,m;k-1,l,m} \phi_{k-1,l,m} + a_{k,l,m;k+1,l,m} \phi_{k+1,l,m} \quad . \tag{2-2-27}
\end{aligned}$$

The coefficients satisfy the following equations:

$$a'_{k,l;k,l} = -a_{k,l;k,l-1} - a_{k,l;k,l+1} - a_{k,l;k-1,l} - a_{k,l;k+1,l} \tag{2-2-28}$$

$$a'_{k,l,m;k,l,m} = -a_{k,l,m;k,l,m-1} - a_{k,l,m;k,l,m+1} - a_{k,l,m;k,l-1,m} - a_{k,l,m;k,l+1,m} - a_{k,l,m;k-1,l,m} - a_{k,l,m;k+1,l,m} \quad . \tag{2-2-29}$$

Firstly k is changed, then l and m are changed, and finally g is changed. The vector of flux, ϕ, satisfies Eq. (2-2-16) through (2-2-19), but the element matrix A_g becomes a matrix whose structure is shown in the following. For a two-dimensional case, it becomes a tri-diagonal block matrix.

$$
A_g = \begin{bmatrix}
A_{1,1} & A_{1,2} & & & & & & \\
A_{2,1} & A_{2,2} & A_{2,3} & & & & 0 & \\
 & \cdot & \cdot & \cdot & & & & \\
 & & \cdot & \cdot & \cdot & & & \\
 & & & A_{l,l-1} & A_{l,l} & A_{l,l+1} & & \\
 & & & & \cdot & \cdot & \cdot & \\
 & 0 & & & & \cdot & \cdot & \cdot \\
 & & & & & & A_{L,L-1} & A_{L,L}
\end{bmatrix} , \qquad (2\text{-}2\text{-}30)
$$

where the element matrix $A_{l,l-1}$ is a diagonal matrix whose element is $a_{k,l;k,l-1}$ and size is K, $A_{l,l+1}$ is a diagonal matrix whose element is $a_{k,l;k,l+1}$ and size is K, and $A_{l,l}$ is a tri-diagonal matrix as shown below:

$$
A_{l,l} = \begin{bmatrix}
a_{1,l;1,l} & a_{1,l;2,l} & & & & & \\
a_{2,l;1,l} & a_{2,l;2,l} & a_{2,l;3,l} & & & & \\
 & \cdot & \cdot & & & & \\
 & & \cdot & \cdot & & & \\
 & & a_{k,l;k-1,l} & a_{k,l;k,l} & a_{k,l;k+1,l} & & \\
 & & & \cdot & \cdot & & \\
 & & & & \cdot & \cdot & \\
 & & & & & a_{K,l;K-1,l} & a_{K,l;K,l}
\end{bmatrix} . \qquad (2\text{-}2\text{-}31)
$$

For a three-dimensional case, the scalar element in the matrix for a two-dimensional case becomes a matrix. The diagonal elements of a tri-diagonal matrix become tri-diagonal, and nondiagonal element matrixes in the tri-diagonal matrix and diagonal element matrixes of the diagonal matrix become diagonal.

When we solve Eq. (2-2-16), characteristics of the matrix A_g are important. Here, we note several important characteristics of A_g. It is a tri-diagonal matrix as already mentioned. As Eqs. (2-2-10) through (2-2-12) and (2-2-21) show, the diagonal elements are all positive, and nondiagonal elements are all negative. The absolute value of diagonal element is more than the sum of all absolute values of nondiagonal elements in the same row. This characteristic is called a *diagonal dominant*.

In the previous descriptions, the way of defining meshes starts from discretizing each coordinate which is orthogonal to any other coordinate. This is the most popular way, but other ways are also possible. A hexagonal arrangement is often used for a dense configuration of fuel pins. For this arrangement, triangular mesh is usually employed. The matrix A_g can be derived by the similar way described above. The triangular mesh leads to a hexa-diagonal matrix, which is also diagonal dominant.

(2-2-2) Solution of Diffusion Equation

(2-2-2-1) Power Method for Outer Iteration

By introducing discretization approximation to the multigroup diffusion equation (2-1-68), the following matrix equation (2-2-16) is obtained:

$$T\phi = \frac{1}{k_{eff}} M\phi \quad . \tag{2-2-32}$$

This is apparently an eigenvalue equation, and k_{eff} is an eigenvalue and ϕ is an eigenvector. By denoting k_n as the n-th eigenvalue and ψ_n as the corresponding eigenvector, the following equation holds:

$$T\psi_n = \frac{1}{k_n} M\psi_n \quad , \qquad\qquad n=1, \ldots, N \tag{2-2-33}$$

where N is the size of matrix T, and for total energy group of G and total space mesh number of K,

$$N = G \times K \quad . \tag{2-2-34}$$

Eq. (2-2-32) has many solutions as shown by Eq. (2-2-33), but only the largest k_n is the effective neutron multiplication factor k_{eff}. For this value the eigenvector takes all positive elements, and becomes proportional to neutron flux: namely,

$$\phi = \alpha\psi_1 \quad . \tag{2-2-35}$$

The most popular method to obtain k_{eff} and ϕ is the power method. It is already described in Sec. (2-1-5-3). It employs the following iteration scheme:

$$T\phi^{(i+1)} = \frac{1}{k^{(i)}} M\phi^{(i)} \quad , \tag{2-2-36}$$

and

$$k^{(i+1)} = \frac{S^{(i+1)}}{S^{(i)}} k^{(i)} \quad , \tag{2-2-37}$$

where $S^{(i)}$ is the number of total fission neutrons produced by the i-th iteration, and calculated by the following equation:

$$S^{(i)} = vF^T \phi^{(i)} \tag{2-2-38}$$

where v is a vector whose element is the volume of each space mesh. The matrix F is a matrix

defined by Eq. (2-2-24).

In the following the convergence characteristics of this method will be mentioned. The solution $\phi^{(i)}$ at the i-th iteration of Eq. (2-2-36) can be written as:

$$\phi^{(i)} = \frac{1}{\prod\limits_{i'=1}^{i-1} k^{(i')}} (T^{-1}M)^i \phi^{(0)} \quad , \tag{2-2-39}$$

where $\phi^{(0)}$ and $k^{(0)}$ are initial guesses. The set of eigenvectors ψ_n is complete, and $\phi^{(0)}$ can be expanded as:

$$\phi^{(0)} = \sum_{n=1}^{N} a_n \psi_n \quad . \tag{2-2-40}$$

By substituting this equation into (2-2-39), we obtain:

$$
\begin{aligned}
\phi^{(i)} &= \frac{1}{\prod\limits_{i'=1}^{i-1} k^{(i')}} (T^{-1}M)^i \sum_{n=1}^{N} a_n \psi_n \\
&= \sum_{n=1}^{N} a_n \frac{1}{\prod\limits_{i'=0}^{i-1} k^{(i')}} (T^{-1}M)^i \psi_n \\
&= \sum_{n=1}^{N} a_n \frac{k_n^{\,i}}{\prod\limits_{i'=0}^{i-1} k^{(i')}} \psi_n \quad .
\end{aligned}
\tag{2-2-41}
$$

Since k_1 is the eigenvalue whose absolute value is the maximum in the all eigenvalues, $\phi^{(i)}$ converges to the following value when i tends to infinity:

$$\phi^{(i)} \to \alpha \psi_1 = \phi \quad . \tag{2-2-42}$$

At the same time $k^{(i)}$ converges to $k_1 = k_{eff}$.

The iteration can not continue infinitely, and we must stop the iteration in finite times. The error caused by the stop of iteration in finite times is called *truncation error*. The speed of the convergence depends on the difference between k_1 and k_2, which is called *separation of eigenvalue*. When the number of meshes increases or the group constants $D_g / \Sigma_{f,g}$ becomes smaller, the separation of eigenvalue becomes smaller and the convergence feature becomes worse. It is also important for the stability of the spatial mode.

Sometimes the higher modes need to be solved. *Wielandt iteration method*, which is shown below, is often employed to obtain the higher modes:

$$(T - \frac{1}{k'}M)\phi^{(i+1)} = \frac{1}{h^{(i)}} M\phi^{(i)} \quad , \tag{2-2-43}$$

where

$$\frac{1}{h^{(i)}} = \frac{1}{k^{(i)}} - \frac{1}{k'} \quad . \tag{2-2-44}$$

In these iterations, of course, it is not necessary to calculate $k^{(i)}$. By the similar discussion employed for the power method, in the Wielandt iteration method, the largest eigenvalue of h and the corresponding engenvector. Since h is the largest eigenvalue, the corresponding k, which is calculated by Eq. (2-2-44), is the k nearest to k'. From these discussions, we can derive the method to obtain an eigenvalue k near the value k'. In this method, we simply employ the iteration scheme (2-2-43) and obtain k from converged h and Eq. (2-2-44). We can see that the iteration (2-2-36) is the case for $k' = \infty$ of the Wielandt iteration.

(2-2-2-2) Gaussian Elimination and Choleski's Method

In the above discussion, if Eq. (2-2-36) can be solved, the problem is solved. The right hand side of this equation is known. Therefore our problem finally becomes to solve the following equation:

$$T\phi = s \quad . \tag{2-2-45}$$

By substituting Eq. (2-2-17), it becomes:

$$A\phi = S\phi + s \quad . \tag{2-2-46}$$

It can be rewritten as the following for each energy group:

$$A_g \phi_g = \sum_{g'=1}^{g-1} S_{g',g} \, \phi_{g'} + S_g \quad , \qquad g=1, \ldots, G, \tag{2-2-47}$$

where the upscattering is assumed to be zero as the same way for Eq. (2-2-19). Since the left hand side does not contain ϕ_g, it can be written as:

$$A_g \phi_g = b_g \tag{2-2-48}$$

When we have to treat upscattering, we need to employ the power method for that part. Even in that case we should solve Eq. (2-2-48).

(2-2-2-2-1) Gaussian Elimination

In the following, we discuss the methods for solving Eq. (2-2-48). For simplicity we will omit the suffix g and write the following equation:

$$A\phi = b \quad . \tag{2-2-49}$$

Here the matrix A is assumed to be diagonal or block diagonal given by Eq. (2-2-20) or (2-2-30).

One of the simplest methods to solve Eq. (2-2-49) is an elimination method. Although there are several elimination methods, here we discuss *Gaussian elimination*, whose procedure is very simple and the amount of calculation is small. The calculation procedure for the tri-diagonal case, whose coefficients are given by Eq. (2-2-20), is mentioned below. At first the first equation is

multiplied by $-c_1/d_1$ and added to the second equation. Then, the coefficient of ϕ_1 becomes zero as follows:

$$(d_2 - \frac{c_1}{d_1}e_1)\phi_2 + e_2\phi_3 = b_2 - \frac{c_1}{d_1}b_1 \quad . \tag{2-2-50}$$

In the following, the change of coefficients shown below is performed:

$$d_k = d_k - \frac{c_{k-1}}{d_{k-1}}e_{k-1} \quad , \tag{2-2-51}$$

$$b_k = b_k - \frac{c_{k-1}}{d_{k-1}}b_{k-1} \quad . \tag{2-2-52}$$

These two equations are not conventional equations, but mean the replacement of the right hand side by the left hand side. By performing this replacement from $k=1$ to K, all the elements c_k of the matrix A are erased and the matrix becomes two-diagonal matrix constructed with d_k and e_k. The equation now has the following form:

$$d_k\phi_k + e_k\phi_{k+1} = b_k \quad . \tag{2-2-53}$$

The procedure by this stage is called *forward reduction*. The equation for $k = K$ is given by

$$d_K\phi_K = b_K \quad . \tag{2-2-54}$$

This equation can be solved easily as:

$$\phi_k = \frac{b_k}{d_k}. \tag{2-2-55}$$

By substituting this equation to Eq. (2-2-53) for $k = K - 1$, we can obtain ϕ_{K-1}. Generally we obtain ϕ_k by substituting ϕ_{k+1} to Eq. (2-2-53) or the following equation from $k = K - 1$ to $k = 1$:

$$\phi_k = \frac{b_k - e_k\phi_{k+1}}{d_k} \quad . \tag{2-2-56}$$

This procedure is called *backward substitution*.

When the matrix A is a block tri-diagonal matrix given by Eq. (2-2-30), the following equation can be obtained for forward reduction:

$$A_{l,l} = A_{l,l} - A_{l,l-1}A_{l-1,l-1}^{-1}A_{l-1,l} \quad , \tag{2-2-57}$$

$$b_l = b_l - A_{l,l-1}A_{l-1,l-1}^{-1}b_{l-1} \quad ,$$

and for backward substitution:

$$\phi_l = A_{l,l}^{-1}(b_l - A_{l,l+1}\phi_{l+1}) \quad . \tag{2-2-58}$$

When the matrix A is tri-diagonal, the method shown above is very useful with small memories. However, when nonzero-element exists in other places, even if the number of this kind of elements is small, we may have to treat many other zero-elements, and much memory is required. *Round-off errors* (the errors caused by using a number specified by *n* correct digits to approximate a number which requires more than *n* digits for its exact specification) are large for this method. Therefore, when multi-dimensional diffusion equation with many meshes, it is usually solved by the SOR method mentioned in the next section.

(2-2-2-2-2) Choleski's Method

In the previous section, the matrix is assumed tri-diagonal. If the matrix does not take such a sparse form and most elements of the matrix are non-zero, required time and memory become very large. When a matrix *A* of Eq. (2-2-49) is such a matrix but positive definite and symmetric, Choleski's method is sometimes employed to reduce these amounts.

The Choleski's method is based on decomposition of the matrix *A* into upper and lower triangular matrices, which are symmetric to each other. Here we will skip the theory of this method, but show only its algorithm. The *l, m*-element of the matrix *A* is denoted as $a_{l,m}$. The algorithm of Choleski's method is given by the following equations:

for forward reduction:

$$a'_{1,1} = \sqrt{a_{1,1}} \quad ,$$

$$a'_{1,m} = \frac{a_{1,m}}{a'_{1,1}} \quad , \qquad \text{for } m=1, \dots, L,$$

$$b'_1 = \frac{b_1}{a'_{1,1}} \quad ,$$

$$\left.
\begin{aligned}
a'_{l,l} &= \sqrt{a_{l,l} - \sum_{k=1}^{l-1}\left(a'_{k,l}\right)^2} \quad , \\
a'_{l,m} &= \frac{a_{l,m} + \displaystyle\sum_{k=1}^{l-1} a'_{k,l} a'_{k,m}}{a'_{l,l}} \quad , \quad \text{for } m = l+1, \dots, L, \\
b'_l &= \frac{b_l - \displaystyle\sum_{k=1}^{l-1} a'_{k,l} b'_k}{a'_{l,l}} \quad ,
\end{aligned}
\right\} \quad \text{for } l = 2, 3 \dots, L \,,$$

for backward substitution:

$$\phi_L = \frac{b'_L}{a'_{L,L}} \quad ,$$

$$\phi_l = \frac{b'_l - \sum_{k=l+1}^{L} a'_{l,k} \phi_k}{a'_{l,l}} \quad , \quad \text{for } l=n\text{-}1, n\text{-}2, \ldots, 1,$$

(2-2-2-3) Jacobi's Method and SOR Method

In this section, another method to solve Eq. (2-2-49) is described. Methods described in this section are all iterative methods. Iterative methods can usually be written as:

$$\phi^{(i+1)} = H\phi^{(i)} + g \quad , \tag{2-2-59}$$

where the matrix H is called *iteration matrix*. If this iteration is proper, for $i \to \infty$:

$$\phi^{(i+1)} \approx \phi^{(i)} \to \phi \quad . \tag{2-2-60}$$

Therefore, from Eqs. (2-2-59) and (2-2-60):

$$\phi = (I - H)^{-1} g \quad . \tag{2-2-61}$$

Truncation error, which is already mentioned for the power method, should be considered in this kind of method.

(2-2-2-3-1) Jacobi's Method and Gauss-Seidel Method

In the following, a method to find an iteration matrix is discussed. First, the matrix A is discomposed into lower left triangle matrix $-L$, diagonal matrix D, and upper right triangle matrix $-U$: namely,

$$A = -L + D - U \quad . \tag{2-2-62}$$

As a simple iteration method to solve Eq. (2-2-49), the following method can be considered:

$$\phi^{(i+1)} = D^{-1}(b + L\phi^{(i)} + U\phi^{(i)}) \quad . \tag{2-2-63}$$

This method is called *Jacobi's method*. The iteration matrix is written as:

$$H_J = D^{-1}(L + U) \quad . \tag{2-2-64}$$

It is not used for most problems, since its convergence is slow. In solving Eq. (2-2-63), ϕ in $L\phi$ is known. Replacing $L\phi^{(i)}$ by $L\phi^{(i+1)}$ usually make the convergence fast:

$$\phi^{(i+1)} = D^{-1}(b + L\phi^{(i+1)} + U\phi^{(i)}) \quad . \tag{2-2-65}$$

This method is called *Gauss-Seidel method*. The convergence condition for this method is known almost the same as Jacobi's method, though its convergence speed is faster. The iteration matrix of this method will be discussed in the next section.

(2-2-2-3-2) SOR Method

We define the modification amount of the flux by the method at the *i*-th iteration as:

$$\Delta\phi^{(i)} \equiv \phi^{(i+1)} - \phi^{(i)} \quad . \tag{2-2-66}$$

When $\Delta\phi^{(i)}$ is obtained by some method, a method to multiply it by ω and to modify the flux by using this amount can be considered as:

$$\phi^{(i+1)} = \phi^{(i)} + \omega(\phi^{(i+1/2)} - \phi^{(i)}) = (1-\omega)\phi^{(i)} + \omega\phi^{(i+1/2)} \quad , \tag{2-2-67}$$

where the solution before ω multiplication is denoted by $\phi^{(i+1/2)}$. Though it does not always improve the acceleration characteristics, it improves usually for Gauss-Seidel method. This method is called *SOR (successive overrelaxation) method*, and ω is called *overrelaxation factor* or *acceleration factor*. The iteration equation can be written as follows from Eqs. (2-2-65) and (2-2-67):

$$\phi^{(i+1)} = (1-\omega)\phi^{(i)} + \omega D^{-1}(b + L\phi^{(i+1)} + U\phi^{(i)}) \quad . \tag{2-2-68}$$

Here $\phi^{(i+1)}$ in Eq. (2-2-65) is $\phi^{(i+1/2)}$ in Eq. (2-2-67). We rewrite Eq. (2-2-68) in the form of Eq.(2-2-59):

$$\phi^{(i+1)} = (D - \omega L)^{-1}[\{(1-\omega)D + \omega U\}\phi^{(i)} + \omega b] \quad . \tag{2-2-69}$$

The iteration matrix $H(\omega)$ is written as:

$$H(\omega) \equiv (D - \omega L)^{-1}\{(1-\omega)D + \omega U\} \quad , \tag{2-2-70}$$

and Eq. (2-2-69) is written as:

$$\phi^{(i+1)} = H(\omega)\phi^{(i)} + g(\omega) \quad , \tag{2-2-71}$$

where

$$g(\omega) \equiv \omega(D - \omega L)^{-1}b \quad . \tag{2-2-72}$$

The iteration matrix of Gauss-Seidel method can be written as $H(1)$.

In the next section, we discuss the convergence characteristics of the SOR method. When we use Eq. (2-2-71), $\phi^{(i)}$ can be written by using $\phi^{(0)}$ as:

$$\phi^{(i)} = H(\omega)^k \phi^{(0)} + (H(\omega)^{k-1} + \cdots\cdots + H(\omega)^2 + I)g(\omega)$$

$$= H(\omega)^k \, \phi^{(0)} + (I - H(\omega))^{-1} (I - H(\omega)^k) g(\omega) \quad . \tag{2-2-73}$$

When $i \to \infty$, $\phi^{(i)}$ converges to:

$$\phi^{(\infty)} = (I - H(\omega))^{-1} g(\omega) \quad , \tag{2-2-74}$$

if $\|H(\omega)\| < 1$, where $\|H(\omega)\|$ is the *norm* of $H(\omega)$. $\phi^{(\infty)}$ satisfies Eq. (2-2-61) and the solution of Eq. (2-2-49). Therefore, in order to investigate the convergence of SOR method, it is necessary to check $\|H(\omega)\|$. In this textbook, I omit the description about the norm, since we do not have an enough space. If you want to study more about basic mathematics useful for the numerical analysis, read Ref. (1). It may be better for readers to know several kinds of norms. The following are well known:

For a matrix

$$A \equiv \begin{bmatrix} a_{1,1} & \cdots & & & \cdots & a_{1,L} \\ \vdots & \ddots & & & & \vdots \\ & & a_{l,l} & a_{l,l+1} & & \\ & & a_{l+1,l} & a_{l+1,l+1} & & \\ \vdots & & & & \ddots & \vdots \\ a_{L,1} & \cdots & & & \cdots & a_{L,L} \end{bmatrix} \tag{2-2-75}$$

l_1 norm: $\qquad \|A\|_1 \equiv \max_{1 \le l \le L} \sum_{k=1}^{L} |a_{k,l}| \tag{2-2-76}$

l_2 norm: $\qquad \|A\|_2 \equiv \left[\rho(A^T A) \right]^{1/2} \tag{2-2-77}$

l_∞ norm: $\qquad \|A\|_\infty \equiv \max_{1 \le k \le L} \sum_{l=1}^{L} |a_{k,l}| \tag{2-2-78}$

where $\rho(B)$ is the spectral radius of matrix B, and defined as:

$$\rho(B) \equiv \max_{1 \le l \le L} (|\lambda_l|) \quad , \tag{2-2-79}$$

where λ_l is the eigenvalue of matrix B.

The asymptotic convergence factor of iteration (2-2-59) is $\rho(H)$. If H_J has a p-fold zero eigenvalue, then $H(\omega)$ has p corresponding eigenvalues equal to $1 - \omega$. Moreover, associated with the $2r$ nonzero eigenvalues $\pm \mu_i$ of H_J are $2r$ eigenvalues, λ_i, of $H(\omega)$ which satisfy:

$$(\lambda_i + \omega - 1)^2 = \lambda_i \omega^2 \mu_i^2 \quad . \tag{2-2-80}$$

For the Gauss-Seidel method, $\omega = 1$ and μ_i^2 are its eigenvalues. The asymptotic convergence

factor of SOR iteration is obtained by solving λ_i of Eq. (2-2-80) for the largest eigenvalue, namely spectral radius of Jacobi's iteration μ_i. Obtained solutions are given in Fig. 2-2-1. The minimum value appears at:

$$\omega_0 = \frac{2}{1 + \sqrt{1 - \mu_i^2}} \quad . \tag{2-2-81}$$

For $\omega \leq \omega_0$, λ_i decreases with increasing ω, and for $\omega \geq \omega_0$, λ_i increasing with decreasing ω. The convergence becomes fastest at $\omega = \omega_0$. For $\omega \leq \omega_0$, λ_i is real and the convergence is monotonically, and for $\omega \geq \omega_0$, λ_i is complex and the convergence is oscillatory.
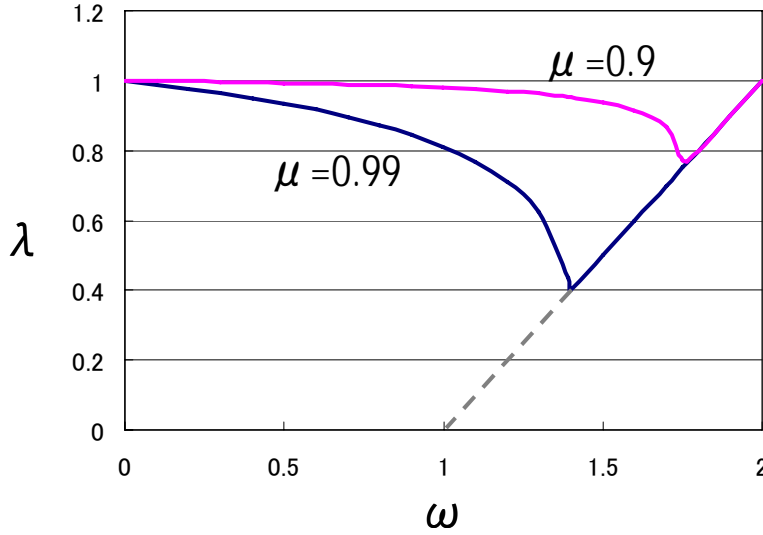
Figure 2-2-1　Asymptotic convergence factor of SOR iteration for given spectral radius of Jacobi's iteration.

The iteration matrix of SOR method is not symmetric, that is:

$$H(\omega)^T \neq H(\omega) \quad . \tag{2-2-82}$$

In many cases a symmetric matrix usually shows better convergence characteristics. Here we will discuss a little bit of symmetrization of SOR iteration matrix. A simple way is changing the direction of solving equations so that after solving from top to bottom, next solving from bottom to top and then from top to bottom and so on. The iteration matrix is written as:

$$H_S(\omega) = (D - \omega L)^{-1}[(1 - \omega)D + \omega U] \times (D - \omega U)^{-1}[(1 - \omega)D + \omega L] \quad . \tag{2-2-83}$$

This iteration method is called SSOR method. However, the speed of convergence of this method is usually slower than the original SOR method, and it is not widely used.

As a method connecting SOR method and SSOR method, the following method is

proposed:

$$H_U(\omega) = (D - \omega L)^{-1}[(1-\omega)D + \omega U] \times (D - \theta U)^{-1}[(1-\theta)D + \theta L] \quad . \tag{2-2-84}$$

This iteration method is called USOR method. When $\theta = 0$, it becomes the SOR method, and $\theta = 1$, it becomes the SSOR method. The optimum value of θ is considered to exist. This method is not widely used either.

(2-2-2-4) Chebyshev (Tchebyshev) Acceleration

We again consider the iteration scheme given by Eq. (2-2-59). Here the error at the i-th iteration, $e^{(i)}$, is given by:

$$e^{(i)} = \phi^{(i)} - \phi^* \quad , \tag{2-2-85}$$

where ϕ^* is the exact solution and satisfies the following equation:

$$\phi^* = H\phi^* + g \quad . \tag{2-2-86}$$

From Eqs. (2-2-59), (2-2-85) and (2-2-86), we obtain the following equation for the error:

$$e^{(i+1)} = He^{(i)} \quad . \tag{2-2-87}$$

The matrix H is assumed to satisfy the following eigenvalue equation:

$$H\psi_n = \lambda_n \psi_n \quad , \qquad n=1, 2, \ldots, N \,, \tag{2-2-88}$$

where we assume all the eigenvalues are real. The Chebyshev acceleration does not work well for the case of complex eigenvalues. We should note that they are real for Jacobi's method but complex for SOR method. We also assume ψ_n consists a complete set.

Here we assume for large enough I and $i>I$ the characteristics of iteration become steady. We correct the $(I+j)$-th solution by the following equation:

$$\phi^{(I+j)+} = \sum_{k=0}^{j} a_{j,k} \phi^{(I+k)} \quad , \tag{2-2-89}$$

where $\phi^{(I+j)}$ is a solution obtained by the previous iteration method, and $\phi^{(I+j)+}$ is a solution for the present method. By using Eq. (2-2-59), $\phi^{(I+k)}$ can be calculated as:

$$\begin{aligned}
\phi^{(I+k)} &= H^k \phi^{(I)} + \sum_{h=0}^{k-1} H^h g \\
&= H^k \phi^{(I)} + (I-H)^{-1}(I - H^k)g \quad .
\end{aligned} \tag{2-2-90}$$

By substituting Eq. (2-2-90) into Eq. (2-2-89), $\phi^{(I+j)+}$ can be written as:

$$\phi^{(I+j)+} = \sum_{k=0}^{j} a_{j,k} H^k \phi^{(I)} + (I-H)^{-1} \sum_{k=0}^{j} a_{j,k} (I-H^k) g \quad . \tag{2-2-91}$$

Next, by substituting Eq. (2-2-85) into Eq. (2-2-89), we obtain:

$$\phi^* + e^{(I+j)+} = \phi^* \sum_{k=0}^{j} a_{j,k} + \sum_{k=0}^{j} a_{j,k} e^{(I+k)} \quad . \tag{2-2-92}$$

Since $e^{(i)}$ is the error and converges to zero, we find:

$$\sum_{k=0}^{j} a_{j,k} = 1 \quad , \tag{2-2-93}$$

and

$$e^{(I+j)+} = \sum_{k=0}^{j} a_{j,k} e^{(I+k)} \quad . \tag{2-2-94}$$

Therefore, the problem becomes finding a proper set of $a_{j,k}$ to minimize $\sum_{k=0}^{j} a_{j,k} e^{(I+k)}$ under the condition (2-2-93). By substituting Eq. (2-2-87) into Eq. (2-2-94):

$$e^{(I+j)+} = \sum_{k=0}^{j} a_{j,k} H^k e^{(I)} \quad . \tag{2-2-95}$$

Here, $e^{(I)}$ can be expanded by ψ_n, since ψ_n is a completed set:

$$e^{(I)} = \sum_{n=1}^{N} c_n \psi_n \quad . \tag{2-2-96}$$

By substituting Eq. (2-2-96) into Eq. (2-2-95):

$$
\begin{aligned}
e^{(I+j)+} &= \sum_{k=0}^{j} a_{j,k} H^k \sum_{n=1}^{N} c_n \psi_n \\
&= \sum_{k=0}^{j} a_{j,k} \sum_{n=1}^{N} c_n \lambda_n^{\ k} \psi_n \\
&= \sum_{n=0}^{N} c_n \sum_{k=1}^{j} a_{j,k} \lambda_n^{\ k} \psi_n \\
&= \sum_{n=0}^{N} c_n P_j(\lambda_n) \psi_n \quad ,
\end{aligned} \tag{2-2-97}
$$

where

$$P_j(\lambda_n) = \sum_{k=0}^{j} a_{j,k} \lambda_n^{k} \quad . \tag{2-2-98}$$

Now the problem can be written in the following way:
For the condition

$$P_j(1) = 1 \quad , \tag{2-2-99}$$

which is equivalent to the condition (2-2-93), minimize:

$$\max_{\lambda_n} P_j(\lambda_n) \tag{2-2-100}$$

by choosing proper $a_{j,k}$.

Since all eigenvalues λ_n are difficult to be obtained, we change Eq. (2-2-100) to:

$$\max_{\lambda_{min} \le \lambda \le \lambda_{max}} P_j(\lambda) \quad , \tag{2-2-101}$$

where λ_{min} and λ_{max} are the minimum and maximum values of λ_n. The problem is to find a proper $a_{j,k}$ to minimize Eq. (2-2-101).

Chebyshev (Tchebyshev) polynomials, $T_j(\phi)$, minimizes:

$$\max \sum_{k=0}^{j} b_{j,k} \phi^k \quad , \qquad \text{for } -1 \le \phi \le 1. \tag{2-2-102}$$

Therefore, $P_j(\lambda)$ can be written by using Chebyshev polynomials as:

$$P_j(\lambda) = \frac{T_j(e\lambda - f)}{T_j(e - f)} \quad , \tag{2-2-103}$$

where:

$$e = \frac{2}{\lambda_{max} - \lambda_{min}} \quad , \tag{2-2-104}$$

$$f = \frac{\lambda_{max} + \lambda_{min}}{\lambda_{max} - \lambda_{min}} \quad . \tag{2-2-105}$$

Chebyshev polynomials satisfy the following recurrence formula:

$$T_{j+1}(\phi) = 2\phi T_j(\phi) - T_{j-1}(\phi) \quad . \tag{2-2-106}$$

Therefore, $P_j(\lambda)$ satisfies the following recurrence formula:

$$P_{j+1}(\lambda) = \frac{e\lambda - f}{e - f}(1 + \mu_j)P_j(\lambda) - \mu_j P_{j-1}(\lambda) \quad , \tag{2-2-107}$$

where:

$$\mu_j = \frac{T_{j-1}(e - f)}{T_{j+1}(e - f)} \quad . \tag{2-2-108}$$

Eq. (2-2-91) can be written as:

$$\phi^{(I+j)+} = P_j(H)\phi^{(I)} + (I - H)^{-1}(1 - P_j(H))g \quad . \tag{2-2-109}$$

From Eqs. (2-2-107) and (2-2-109) we obtain the following recurrence formula for $\phi^{(I+j)+}$:

$$\phi^{(I+j+1)+} = \frac{eH - f}{e - f}(1 + \mu_j)\phi^{(I+j)+} - \mu_j\phi^{(I+j-1)+} + \frac{e}{e - f}(1 + \mu_j)g \quad . \tag{2-2-110}$$

Here we summarize the procedure of this method. At first we repeat iteration by using the iteration matrix H until the characteristic of convergence becomes stable. When it becomes stable, calculate e and f by using $\lambda_{\min}$ and $\lambda_{\max}$, and Eqs. (2-2-104) and (2-2-105). Calculate μ_j for each iteration time j by using Eq. (2-2-108), and repeat Eq. (2-2-110) to obtain $\phi^{(I+j+1)+}$. Generally $\lambda_{\min}$ and $\lambda_{\max}$ are difficult to obtain. The spectral radius, ρ, of H may be estimated easily in an acceptable accuracy through the iterative calculations by the I-th iteration. When ρ is given, we may replace $\lambda_{\min}$ and $\lambda_{\max}$ by $-\rho$ and ρ. For this case:

$$e = \rho \, ,$$

$$f = 0 \, ,$$

and the equation becomes simple. When all the eigenvalues are positive, we can set:

$$\lambda_{\min} = 0 \quad .$$

(2-2-2-5) SD Method and CG Method

We consider another iteration method to solve Eq. (2-2-49) by using the following iteration scheme:

$$\phi^{(i+1)} = \phi^{(i)} + \alpha^{(i)}\theta^{(i)} \quad , \tag{2-2-111}$$

where $\theta^{(i)}$ is the direction of correction and $\alpha^{(i)}$ is the magnitude of correction. Since the exact solution ϕ^* is not known, the error of $\phi^{(i)}$:

$$s^{(i)} \equiv \phi^{(i)} - \phi^* \tag{2-2-112}$$

is unknown. However, the error of b defined by:

$$r^{(i)} \equiv A\phi^{(i)} - b \tag{2-2-113}$$

can be calculated. $r^{(i)}$ can also be written as:

$$r^{(i)} = A\left(\phi^{(i)} - \phi^*\right) \tag{2-2-114}$$

$$= As^{(i)} \ . \tag{2-2-115}$$

We consider the following function:

$$f(\phi) \equiv r^T r$$

$$= (A\phi - b)^T (A\phi - b). \tag{2-2-116}$$

It takes its minimum value, 0, at $\phi = \phi^*$. The equation $f(\phi) = \text{constant}$ shows an ellipse in multidimensional space, whose center is $\phi = \phi^*$. Our problem is equivalent to find the center of this ellipse. From this discussion, we try to find $\theta^{(i)}$ directing to this center.

We consider the case that the matrix A is a positive definite and symmetric. For this case, not $f(\phi)$ but the following function is usually minimized:

$$g(\phi) \equiv r^T A^{-1} r \ . \tag{2-2-117}$$

$g(\phi)$ can be rewritten as:

$$g(\phi) = (A\phi - b)^T A^{-1}(A\phi - b)$$

$$= (\phi - A^{-1}b)^T A(\phi - A^{-1}b)$$

$$= (\phi - \phi^*)^T A(\phi - \phi^*)$$

$$= s^T As \ . \tag{2-2-118}$$

Since A is a positive definite, $g(\phi)$ is always positive and takes its minimum value, 0, at $\phi = \phi^*$. The treatment of Eq. (2-2-117) is much easier than Eq. (2-2-116), and then we will treat Eq. (2-2-117) in the following. Even if A is not positive definite and symmetric, we can make the problem $A\phi = b$ positive definite and symmetric by multiplying the matrix A^T on both sides of the equation:

$$A^T A\phi = A^T b \ . \tag{2-2-119}$$

We have two methods based on this idea: *SD (steepest descent) method* and *CG (conjugate gradients) method*. SD method is not widely used compared with CG method. However, since it

is more basic and simple, we will start discussion on SD method.

(2-2-2-5-1) SD Method

Since we try to minimize the amount of $g(\phi)$, the direction $\theta^{(i)}$ may be better chosen to reduce the amount of $g(\phi^{(i)})$ most. Such direction is opposite to the direction of gradient of $g(\phi^{(i)})$: namely,

$$\theta^{(i)} = -\beta \nabla g(\phi^{(i)})$$

$$= -2\beta(A\phi^{(i)} - b)$$

$$= -2\beta r^{(i)} \quad ,$$

where β is an arbitrary constant, and we choose $\beta = -1/2$. Therefore, we choose:

$$\theta^{(i)} = r^{(i)} \quad . \tag{2-2-120}$$

In the next step, we will fix $\alpha^{(i)}$ in Eq. (2-2-111). In SD method, it is chosen to minimize $g(\phi^{(i+1)})$, where $\phi^{(i+1)}$ is given by Eq. (2-2-111), so that:

$$\frac{\partial}{\partial \alpha} g(\phi + \alpha \theta) = 0 \quad . \tag{2-2-121}$$

Here

$$\frac{\partial}{\partial \alpha} g(\phi + \alpha r) = \frac{\partial}{\partial \alpha}[A(\phi + \alpha r) - b]^T A^{-1}[A(\phi + \alpha r) - b]$$
$$= 2(r^T A r \alpha + r^T r) \quad . \tag{2-2-122}$$

From Eqs. (2-2-121) and (2-2-122), we choose $\alpha^{(i)}$ as:

$$\alpha^{(i)} = -\frac{r^{(i)T} r^{(i)}}{r^{(i)T} A r^{(i)}} \quad . \tag{2-2-123}$$

Therefore, Eq. (2-2-111) becomes the following equation for SD method:

$$\phi^{(i+1)} = \phi^{(i)} - \frac{r^{(i)T} r^{(i)}}{r^{(i)T} A r^{(i)}} r^{(i)} \quad . \tag{2-2-124}$$

(2-2-2-5-2) CG Method

We discuss CG method also for a positive definite symmetric matrix A. The way to transform any matrix to satisfy this condition has been already mentioned (See Eq. (2-2-119)). In the SD method, the correction factor α is chosen to minimize $g(\phi + \alpha \theta)$ on the line determined by direction θ. This method depends on local information and is not always

optimum. In the CG method, we try to find the solution using global information.

In this method, $\theta^{(i+1)}$ is chosen orthogonal to any $\theta^{(j)}$ for $j=1,\ldots,I$, and then the component of the error belonging to this direction is deleted. If this procedure is continued successfully, the error becomes zero by i becoming L, the dimension of the matrix A. Since we consider the minimization of Eq. (2-2-117), here we use *A-orthogonal* for definition of orthogonal, where x and y are orthogonal to each other, which means:

$$x^T A y = 0 \ . \tag{2-2-125}$$

As already mentioned, $\theta^{(i+1)}$ is chosen orthogonal to any $\theta^{(j)}$ for $j=1,\ldots,i$: namely;

$$\theta^{(i+1)T} A \theta^{(j)} = 0 \ , \qquad \text{for } j=1,\ldots,i \ . \tag{2-2-126}$$

And since the component of the error belonging to this direction is deleted:

$$[\phi^{(i+1)} - \phi^{(i)}]^T A[\phi^{(i+1)} - \phi^*] = 0 \ , \tag{2-2-127}$$

or

$$\theta^{(i)T} A r^{(i+1)} = 0 \ . \tag{2-2-128}$$

Here $\phi^{(i+1)}$ is chosen so that it locates on the line:

$$\phi^{(i+1)} = \phi^{(i)} + \alpha^{(i)} \theta^{(i)} \ . \tag{2-2-129}$$

By substituting Eq. (2-2-111) into Eq. (2-2-127) we obtain:

$$\alpha^{(i)} \theta^{(i)T} A[\phi^{(i)} - \phi^* + \alpha^{(i)} \theta^{(i)}] = 0 \ .$$

It can be rewritten as:

$$\theta^{(i)T} r^{(i)} + \alpha^{(i)} \theta^{(i)T} A \theta^{(i)} = 0 \ .$$

Therefore we can choose $\alpha^{(i)}$ as:

$$\alpha^{(i)} = -\frac{\theta^{(i)T} r^{(i)}}{\theta^{(i)T} A \theta^{(i)}} \ . \tag{2-2-130}$$

The condition (2-2-126) can be realized if we choose $\theta^{(j+1)}$ for $j=1,\ldots,i$:

$$\theta^{(j+1)T} A \theta^{(j)} = 0 \ , \qquad \text{for } j=1,\ldots,i \ . \tag{2-2-131}$$

Therefore, we choose the form of $\theta^{(i+1)}$ as:

$$\theta^{(i+1)} = r^{(i+1)} - \beta^{(i)} \theta^{(i)} \ , \tag{2-2-132}$$

and by substituting this equation in to Eq. (2-2-131) for $j=i$;

$$\left(r^{(i+1)} - \beta^{(i)}\theta^{(i)}\right)^T A\theta^{(i)} = 0 \quad,$$

or

$$\beta^{(i)} = \frac{r^{(i+1)T} A\theta^{(i)}}{\theta^{(i)T} A\theta^{(i)}} \quad. \tag{2-2-133}$$

Now we have obtained all necessary equations for the CG method. At this stage, it is better to summarize the calculation procedure. At the beginning we choose the initial direction $\theta^{(0)}$ as:

$$\theta^{(0)} = A\phi^{(0)} - b = r^{(0)} \quad. \tag{2-2-134}$$

The parameter $\alpha^{(i)}$ is chosen by using Eq. (2-2-129), and $\phi^{(i+1)}$ is calculated by using Eq. (2-2-111). Next we calculate $r^{(i+1)}$ by using the following equation:

$$r^{(i+1)} = r^{(i)} + \alpha^{(i)} A\theta^{(i)} \quad. \tag{2-2-135}$$

This equation can be obtained easily from Eqs. (2-2-111) and (2-2-113). Next the parameter $\beta^{(i)}$ is chosen by using Eq. (2-2-133), and $\theta^{(i+1)}$ is calculated by using Eq. (2-2-132). After that, the procedure will be repeated. Theoretically, as mentioned before, the exact solution can be obtained before the iteration time becomes I. However, in real calculations, it is almost impossible, since round-off errors exist.

Preconditioning of the matrix A may improve the convergence characteristics of the method. When Eq. (2-2-116) is minimized instead of Eq. (2-2-117), the algorithm may be changed. We have many kinds of CG-like methods.[2]

We will see a different kind of application of the CG method to reactor physics problems. The eigenvalue equation (2-2-32) can be solved by minimizing the Rayleigh quotient:

$$R(\phi) = \frac{\phi^T T \phi}{\phi^T M \phi} \quad, \tag{2-2-136}$$

where ϕ^T is usually an adjoint vector to ϕ, and:

$$k_{eff} = \frac{1}{\min_{\phi} R(\phi)} \quad. \tag{2-2-137}$$

Here we can also use CG method for minimization of the Rayleigh quotient.[3]

References

1) J. M. Ortega, "Numerical Analysis," Academic Press, New York (1972).

2) E. Suetomi, H. Sekimoto, Conjugate Gradient Like Methods and Their Application to Fixed Source Neutron Diffusion Problems, J. Nucl. Sci. Technol., 26[10], 913-926(1989).

3) E. Suetomi, H. Sekimoto, Conjugate Gradient Like Methods and Their Application to Eigenvalue Problems for Neutron Diffusion Equation, Ann. Nucl. Energy, 18[4], 205-228(1991).

Problems

Homework 1

1-1. One fission of fissile nucleus such as ^{235}U and ^{239}Pu yields about 200 MeV of energy. Noting that:

　　1 eV = 1.6x10^{-19} J,

　　how many joules are released in the fission of one fissile nucleus?

1-2. Applying Einstein's formula:

　　E = Mc^2,

　　where c = 3x10^8 m/sec, the speed of light, how many kilograms of matter are converted into energy in the previous problem?

1-3. If the atom of ^{235}U and ^{239}Pu has mass of 235amu and 239amu, respectively, what amount of equivalent energy does it have, where 1amu = 931.5MeV/c^2?

1-4. Using the previous results, what fraction of the mass of ^{235}U and ^{239}Pu nucleus is converted into energy when fission takes place?

1-5. How many fission events per second of ^{235}U and ^{239}Pu can produce a thermal power of 1W respectively?

1-6. How many kilograms of ^{235}U and ^{239}Pu are fissioned to produce 3000MW of thermal power (which is equivalent to about 1000MW of electricity) per 1day respectively?

1-7. In the highly developed country such as USA, one average person is consuming energy with the rate of 10kW.   If they use 10% of this energy (nuclear thermal energy) by fissions of ^{235}U and ^{239}Pu, estimate the amount (kg) of ^{235}U and ^{239}Pu he or she has consumed during his or her whole life, where his life is assumed to be 80 years.

1-8. The whole world population in 2050 is estimated to be 9x10^9.   If they will be consuming energy at the rate given in the previous question, what is the amount (kg) of ^{235}U and ^{239}Pu consumed in 100 years respectively?

Homework 2

Problem 2A: fission reaction

1)　　Calculate the atomic mass of ^{235}U by using the equation shown in the textbook, and compare it with the recommended value obtained from the home-page:
< http://wwwndc.tokai-sc.jaea.go.jp/NuC/index_J.html >.

2)　　Consider the following fission reaction of ^{235}U by absorbing a thermal neutron:

$$^{235}U + n \rightarrow {}^{138}Xe + {}^{A}X + 2n + Q$$

2-1) What is ^{A}X?

2-2) Calculate Q in MeV.

2-3) ^{138}Xe and ^{A}X are unstable, and will make β-decays to become the respective stable nuclides.
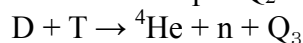   What are these stable nuclides?
    Calculate the energies produced for these decays.

2-4) What is the total energy produced by this fission and associating decays?

Problem 2B: Fusion reaction

Consider the following fusion reactions, where a deuteron with the energy of 50keV is assumed to collide with a target nucleus at rest:

$$D + D \rightarrow {}^{3}He + n + Q_1$$
$$D + D \rightarrow T + p + Q_2$$
$$D + T \rightarrow {}^{4}He + n + Q_3$$
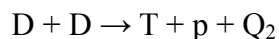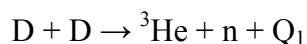
1)   Calculate Q_1, Q_2, Q_3.

2)   Also calculate both maximum and minimum kinetic energies of neutrons produced in the first and third reactions.

Homework 3

Solve the Problems 3A through 3C by using Tables 1 through 4.

Problem 3A:

Calculate the mean free path of the following neutrons:
14MeV (D-T fusion neutron)
Fission neutrons
Thermal neutrons

In the following materials:
Air (nitrogen 78%, oxygen 21%, argon 1%; 1 atm.)
water,
heavy water
graphite
natural uranium metal
^{235}U metal
by using the values given in Tables 1 through 4 and
    Avogadro's number = $0.602252 \times 10^{24} mole^{-1}$

Problem 3B:

Calculate the average number of collisions required for slowing-down from typical energy (1MeV) for fission neutron to thermal energy (0.025eV) in the following pure materials:
proton
deuteron
oxygen
graphite
^{235}U
if only elastic scattering is considered.
Discuss the slowing-down in mixed isotope materials.

Problem 3C:

Calculate the average number of collisions of thermal neutron until absorbed in the following materials:
Air (nitrogen 78%, oxygen 21%, argon 1%; 1 atm.)
water
heavy water
graphite
natural uranium metal
^{235}U metal
where the energy change by scattering is neglected.

Problem 3D:

Calculate the η-value for uranium isotopes for the following neutrons:
14MeV (D-T fusion neutron)
Fission neutrons
Thermal neutrons

Table 1.   Properties of the elements and molecules.

Element or molecule	Atomic or molecular weig	Normal density (g/cm3)
Water	18.0167	1
Heavy water	20.0276	1.105
Graphite	12.01115	1.6
Uranium metal	238.03	19.1

The data for uranium are for the natural uranium. It is accepted to assume that the number density for other uranium composed by different isotopic composition is the same as for the natural uranium.

Table 2.   Microscopic scattering cross section (barns).   (from JENDL-3.2)

	14MeV	Fiss. Av.	Maxw. Av.	0.025eV
1H	0.692	3.99	29	30.1
2H	0.625	2.54	4.15	4.23
12C	0.804	2.37	4.94	4.95
14N	0.984	1.85	10.36	10.37
16O	0.898	2.77	3.9	3.9
40Ar	0.788	2.55	0.655	0.655
235U	2.87	4.6	15	15
238U	2.7	4.85	9.38	9.38

Table 3.   Microscopic absorption cross section (barns).   (from JENDL-3.2)

	14MeV	Fiss. Av.	Maxw. Av.	0.025eV
1H	0	0	0.294	0.332
2H	0	0	0.0005	0.0005
12C	0	0	0.0031	0.0035
14N	0.004	0.034	1.64	1.85
16O	0.044	0	0.0002	0.0002
40Ar	0.015	0	0.585	0.66
235U	2.05	1.33	593.5	683.2
238U	1.14	0.371	2.41	2.72

Table 4.   Microscopic fission cross section (barns).   (from JENDL-3.2)

	14MeV	Fiss. Av.	Maxw. Av.	0.025eV
1H	0	0	0	0
2H	0	0	0	0
12C	0	0	0	0
14N	0	0	0	0
16O	0	0	0	0
40Ar	0	0	0	0
235U	2.05	1.24	506.8	584.4
238U	1.14	0.304	0	0

Homework 4

Consider the material whose group constants are given in Table 1.

Table 1.   5-group Constants.

Group	E_g^{upper}	χ_g	Σ_{ag} (/cm)	Σ_{fg} (/cm)	D (cm)
1	10 MeV	0.9	0.04	0.06	2.5
2	100 keV	0.1	0.06	0.04	1
3	1 keV	0	0.05	0.05	0.9
4	10 eV	0	0.17	0.13	0.8
5	1 eV	0	3	4.4	0.24

$\nu = 2.5$

Scattering Matrix, $\Sigma_{g \to g'}$.

g' \ g	1	2	3	4	5
1	0.22	0	0	0	0
2	0.02	0.54	0	0	0
3	0	0.005	0.76	0	0
4	0	0	0.001	0.56	0
5	0	0	0	0.00005	0.47

where (n,2n) reaction is included in the scattering matrix.
The removal cross section is assumed to be obtained from:

$$\Sigma_{r,g} = \Sigma_{a,g} + \sum_{g'=g+1}^{G} \Sigma_{g \to g'} \quad .$$

Problem 5A:

Calculate the infinite medium neutron multiplication factor, k_{inf} , for this material and corresponding neutron spectrum (use both /lethargy and /eV for its unit), where the neutron spectrum ϕ_g is normalized when the power density is 100W/cm^3.

Problem 5B:

Get one-group constants by using the obtained spectrum as a weighting function and calculate the infinite medium neutron multiplication factor from these one-group constants.

Hint:
At first, calculate ϕ_g by assuming $S/k_{inf} = 1$. Then after calculating S, solve k_{inf} and normalize neutron spectrum.

Homework 5

Considering the same material given in Problem 4, solve the following problems:

Problem 5A:
Calculate the effective neutron multiplication factor for the cylindrical bare reactor by using the 5-group constants, where both radius and height are 1 m and the extrapolation distance should be evaluated for each energy group.

Problem 5B:
Calculate the same quantity by using 1-group constants obtained for Problem 4.

Problem 5C:
Calculate the critical radius of this reactor by using 1-group constants, where the height is 1m.

Problem 5D:
Calculate the critical radius of this reactor by using 5-group constants, where the height is 1m.

Final Examination

Suppose a bare spherical reactor, whose radius is R, in the vacuum space, and solve the following problems:

Problem 1
The neutron flux in the reactor can be assumed to satisfy 2-group diffusion equation.
Write down the neutron diffusion equation using r for radial position and employing the following notations and assumptions:
1) $\Sigma_{f,2}$: Macroscopic fission cross section. Fission occurs only in the 2nd group, and does not occur in the 1st group.
2) ν: Average fission neutron number. All fission neutrons appear in 1st group.
3) $\Sigma_{1 \to 2}$: Macroscopic neutron slowing down cross section from the 1st to 2nd group.
4) $\Sigma_{c,g}$ and D_g: Macroscopic capture cross section and diffusion coefficient for g-group, respectively.
5) k: for effective neutron multiplication factor.
6) The other reactions can be neglected, and neutron acceleration from 2nd to 1st group does not occur.

Problem 2.
Solve the infinite neutron multiplication factor for the following case:
        $\nu=2.5$、$\Sigma_{f,2}=2.0\text{cm}^{-1}$、$\Sigma_{c,1}=0.010\text{cm}^{-1}$、$\Sigma_{c,2}=1.0\text{cm}^{-1}$、$\Sigma_{1 \to 2}=0.030\text{cm}^{-1}$.
Hint: Consider the uniform infinite medium.

Problem 3.
Obtain the critical radius of this bare spherical reactor, where $D_1=1\text{cm}$ and $D_2=0$. The extrapolation distance can be assumed 0 for each energy group.