A Simple Global View of Fuel Burnup

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Abstract. Reactor physics and fuel burnup are discussed in order to obtain a simple global view of the effects of nuclear reactor characteristics to fuel cycle system performance. It may provide some idea of free thinking and overall vision, though it is still a small part of nuclear energy system. At the beginning of this lecture, governing equations for nuclear reactors are presented. Since the set of these equations is so big and complicated, it is simplified by imposing some extreme conditions and the nuclear equilibrium equation is derived. Some features of future nuclear equilibrium state are obtained by solving this equation. The contribution of a nucleus charged into reactor core to the system performance indexes such as criticality is worth for understanding the importance of each nuclide. It is called nuclide importance and can be evaluated by using the equations adjoint to the nuclear equilibrium equation. Examples of some importances and their application to criticality search problem are presented.

1. Introduction

“Free Thinking and Overall Vision” was an important guiding principle of the 21st Century Centre of Excellence (COE) Program “Innovative Nuclear Energy Systems for Sustainable Development of the World” promoted by Tokyo Institute of Technology where I was working as the leader [1]. This guiding principle is considered important not only for the Program but for all peoples involving in nuclear energy. Low operation rates, troubles and accidents met in nuclear power production activities may be attributed to the lack of it.

In the last September on Jeju Island, Korea, I made an invited lecture at the first Reactor Physics Asia Conference (RPHA), where I tried to make the attending reactor physics specialists get some idea of free thinking and overall vision. This lecture has been revised for the present lecture to be desirable for more general audiences.

The present lecture is on reactor physics and fuel burnup. It shows a simple global view of fuel burnup and reactor characteristics. I hope it provides us some ideas of free thinking and overall vision on this field, though it is still a small part of nuclear energy system.

At the beginning of this lecture, governing equations for nuclear reactors are presented. Since the set of these equations is so big and complicated, we try to simplify it by imposing some extreme conditions and to derive the nuclear equilibrium equation. Some features of future nuclear equilibrium state are obtained by solving this equation. The contribution of a nucleus charged into reactor core to the system performance indexes such as criticality is worth for understanding the importance of each nuclide. It is called nuclide importance and can be evaluated by using the equations adjoint to the nuclear equilibrium equation. Examples of some importances and their application to criticality search problem are presented in this lecture.
2. Basic Equations of Neutron Transport and Fuel Burning

2.1. Governing equations
For the investigation of global view of fuel burnup, the main parameters are neutron flux, \( \phi(\vec{r}, \vec{\Omega}, E, t) \), and nuclide number density distributions, \( n_j(\vec{r}, t) \). In order to obtain these values we should treat the equations for the following distributions as governing equations:

(i) Neutron distribution
(ii) Delayed neutron precursor distribution
(iii) Nuclide (actinide, fission product (FP)) distribution
(iv) Temperature and material distribution

The actual equation for each distribution can be written as follows [2]:

\[
\begin{align*}
\frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, \vec{\Omega}, E, t) + \vec{\Omega} \cdot \nabla \phi(\vec{r}, \vec{\Omega}, E, t) + \sum_j n_j(\vec{r}, t) \sigma_{T,j}(E) \phi(\vec{r}, \vec{\Omega}, E, t) \\
= & \int_0^{E'} dE' \int_{4\pi} d\Omega' \sum_j n_j(\vec{r}, t) \sigma_{S,j}(\vec{\Omega}' \rightarrow E') \phi(\vec{r}, \vec{\Omega}' \rightarrow E', t) \\
+ & \frac{1}{4\pi} \int_0^{E'} dE' \int_4 \Omega_{\rho} d\Omega' \sum_j n_j(\vec{r}, t) \chi_i(E) \nu_j(1 - \beta_j) \sigma_{F,j}(E') \phi(\vec{r}, \vec{\Omega}', E', t) \\
+ & \sum_i \frac{\chi_i(E)}{4\pi} \lambda_i \xi_i(\vec{r}, t) \\
+ & s(\vec{r}, \vec{\Omega}, E, t),
\end{align*}
\]

where

\( \sigma_{T,j}(E) \) : microscopic total cross section of nuclide \( j \) for the neutron with energy \( E \),

\( \sigma_{S,j}(\vec{\Omega}' \rightarrow E) \) : microscopic scattering cross section of the nuclide \( j \) for the neutron with energy \( E' \) and direction \( \vec{\Omega}' \) transferred to \( E \) and \( \vec{\Omega} \). This reaction includes any neutron emitting reactions except fission,

\( \sigma_{F,j}(E) \) : microscopic fission cross section of nuclide \( j \) for the neutron with energy \( E \),

\( \nu_j \) : average number of neutrons emitted by the fission of nuclide \( j \),

\( \chi_i(E) \) : prompt fission neutron energy spectrum,

\( \chi_i(E) \) : delayed neutron energy spectrum for precursor \( i \),

\( \beta_j \) : delayed neutron precursor fraction produced by the fission of nuclide \( j \),

\( \lambda_i \) : decay constant of delayed neutron precursor \( i \),

\( c_i(\vec{r}, t) \) : number density of delayed neutron precursor \( i \),

\( s(\vec{r}, \vec{\Omega}, E, t) \) : external neutron source.

Though \( \chi_i(E) \nu_j(1 - \beta_j) \) is a function of the energy of impinging neutron which causes the fission, the expression \( (E') \) in the equation is omitted for simplicity.

(ii) Delayed neutron precursor distribution
\[
\frac{\partial}{\partial t} c_j(\mathbf{r}, t) + \lambda_i c_j(\mathbf{r}, t) = \int_0^\infty dE' \int_{4\pi} d\Omega' \sum_j n_j(\mathbf{r}, t) \beta_{i,j} \nu_j \sigma_{F,j}(E') \phi(\mathbf{r}, \mathbf{\Omega}', E', t),
\]

where \( \beta_{i,j} \) : fraction of delayed neutron precursor \( i \) produced by the fission of nuclide \( j \), which satisfies

\[
\beta_j = \sum_i \beta_{i,j}.
\]

(iii) Nuclide (actinide, FP) distribution

\[
\frac{\partial}{\partial t} n_j(\mathbf{r}, t) = -n_j(\mathbf{r}, t) \left( \lambda_j + \int_0^\infty dE' \sigma_{A,j}(E') \int_{4\pi} \phi(\mathbf{r}, \mathbf{\Omega}', E', t) d\mathbf{\Omega}' \right) + \sum_k n_k(\mathbf{r}, t) \lambda_{k\rightarrow j} + \sum_k n_k(\mathbf{r}, t) \int_0^\infty dE' \sigma_{k\rightarrow j}(E') \int_{4\pi} \phi(\mathbf{r}, \mathbf{\Omega}', E', t) d\mathbf{\Omega}' ,
\]

where

- \( \sigma_{A,j}(E) \) : microscopic absorption cross section of nuclide \( j \) for the neutron with energy \( E \),
- \( \sigma_{k\rightarrow j}(E) \) : microscopic neutron cross section of nuclide \( k \) to be transformed to nuclide \( j \),
- \( \lambda_j \) : decay constant of nuclide \( j \),
- \( \lambda_{k\rightarrow j} \) : decay constant of nuclide \( k \) to be transformed to \( j \).

Here the nuclide \( n \) covers both fuel and FPs. The production of FP from fission can also be treated by equation (4) by choosing \( \sigma_{k\rightarrow j}(E) \) properly.

It should be noted that equation (4) does not include the in-core fuel managements. We need the initial conditions of nuclide number density distributions, \( n_j(\mathbf{r}, 0) \), and/or in-core fuel management rules. About these points we will discuss in the next chapter for a very simple case.

(iv) Temperature and material distribution

In addition to the above equations we consider the equations of temperature and motion of materials. However, these equations depend on the core configuration very much. For example, we should use different equations for different coolant materials such as gas or liquid. Therefore, hereafter we omit to write the actual equations for these distribution. However, the coolant flow distribution affects strongly the temperature distributions, and the temperature distributions affect the effective microscopic cross sections and the material densities and shapes.

2.2. Steady state reactor operation without external source

In the following we consider the steady state reactor operation without external source, and the following equations hold:

\[
\frac{1}{\nu} \frac{\partial}{\partial t} \phi(\mathbf{r}, \mathbf{\Omega}, E, t) = 0 ,
\]

\[
\frac{\partial}{\partial t} c_j(\mathbf{r}, t) = 0 ,
\]
\[ s(\vec{r}, \vec{Q}, E, t) = 0. \]  

In this case the reactor is in a critical state and the external neutron source does not stay in the core. Only time dependent phenomena considered is the burnup.

In this case equations (1) and (2) can be combined to the following equation:

\[
\hat{Q} \cdot \nabla \phi(\vec{r}, \vec{Q}, E, t) + \sum_j n_j(\vec{r}, t) \sigma_{T,j}(E) \phi(\vec{r}, \vec{Q}, E, t) \\
= \int_0^E dE' \int_{4\pi} d\Omega' \sum_j n_j(\vec{r}, t) \sigma_{S,j}(\vec{Q}, \vec{Q}', E' \rightarrow E) \phi(\vec{r}, \vec{Q}', E', t) \\
+ \frac{1}{4\pi k_{ef}(t)} \int_0^E dE' \int_{4\pi} d\Omega' \sum_j n_j(\vec{r}, t) \chi_j(E) \nu_{j,j}(E') \phi(\vec{r}, \vec{Q}', E', t). \]  

(8)

The reactor is usually kept critical by adjusting the control rods. However, it is complicated to implement this procedure in neutron transport equation, and the effective neutron multiplication factor, \( k_{ef}(t) \), is introduced instead. The reactor is controlled to produce its total power output to be equal to the planned value, \( P(t) \):

\[
\Gamma \int_{4\pi} d\vec{r} \int_0^E dE' \int_{4\pi} d\Omega' \sum_j n_j(\vec{r}, t) \sigma_{S,j}(E') \phi(\vec{r}, \vec{Q}', E', t) = P(t), \]  

(9)

where \( \int_{4\pi} \cdot d\vec{r} \) denotes the integration over the whole core.

The basic equations for our study are equations (4), (8) and (9) and the equations for temperature and material distribution. In the following discussions the equations for temperature and material distribution are omitted from the list of equations.

2.3. Homogeneous infinite medium

In the present paper we study on the homogeneous infinite medium, and the following equations hold:

\[ k_{ef}(t) \rightarrow k_{m}(t), \]  

(10)

\[ P(t) \rightarrow p(t). \]  

(11)

where \( k_{m}(t) \) is the infinite medium neutron multiplication factor and \( p(t) \) is the power density. In this case the arguments \( \vec{r} \) and \( \vec{Q} \) disappear and

\[ \hat{Q} \cdot \nabla \phi(\vec{r}, \vec{Q}, E, t) = 0, \]  

(12)

and the following new variable is introduced:

\[ \phi(E, t) \equiv \int \phi(\vec{r}, \vec{Q}, E, t) d\vec{Q}. \]  

(13)

The governing equations become

\[
\sum_j n_j(t) \sigma_{T,j}(E) \phi(E, t) - \sum_j n_j(t) \int_0^E \sigma_{S,j}(E' \rightarrow E) \phi(E', t) dE' \]
\[ = \frac{1}{k_\alpha(t)} \sum_{j} n_j(t) \mathcal{X}_j(E) \int_0^\infty \nu_j \sigma_{F,j}(E') \phi(E',t) dE', \quad (14) \]

\[ \Gamma \sum_{j} n_j(t) \int_0^\infty \sigma_{F,j}(E') \phi(E',t) dE' = p(t), \quad (15) \]

\[ \frac{\partial}{\partial t} n_j(t) = -n_j(t) \left( \lambda_j + \int_0^\infty \sigma_{A,j}(E') \phi(E',t) dE' \right) + \sum_{k} n_k(t) \lambda_{k\rightarrow j} + \sum_{k} n_k(t) \int_0^\infty \sigma_{k\rightarrow j}(E') \phi(E',t) dE'. \quad (16) \]

### 2.4. Integration over neutron energy

For the study of fuel burnup, the variable \( E \) in neutron flux is not important if we can get one-group cross section set. Here we try to integrate equations (14) through (16). At the beginning we define the following one-group constants:

\[ \phi(t) = \int \phi(E,t) dE, \quad (17) \]

\[ \sigma_{A,j} = \sigma_{A,j}(t) = \frac{\int \sigma_{A,j}(E) \phi(E,t) dE}{\int \phi(E,t) dE}, \quad (18) \]

\[ \sigma_{F,j} = \sigma_{F,j}(t) = \frac{\int \sigma_{F,j}(E) \phi(E,t) dE}{\int \phi(E,t) dE}, \quad (19) \]

\[ \sigma_{k\rightarrow j} = \sigma_{k\rightarrow j}(t) = \frac{\int \sigma_{k\rightarrow j}(E) \phi(E,t) dE}{\int \phi(E,t) dE}. \quad (20) \]

Then equations (14) through (16) can be rewritten as follows:

\[ \sum_{j} n_j(t) \sigma_{A,j} \phi(t) = \frac{1}{k_\alpha(t)} \sum_{j} n_j(t) \nu_j \sigma_{F,j} \phi(t), \quad (21) \]

\[ \Gamma \sum_{j} n_j(t) \sigma_{F,j} \phi(t) = p(t), \quad (22) \]

\[ \frac{\partial}{\partial t} n_j(t) = -n_j(t) \left( \lambda_j + \sigma_{A,j} \phi(t) \right) + \sum_{k} n_k(t) \lambda_{k\rightarrow j} + \sum_{k} n_k(t) \sigma_{k\rightarrow j} \phi(t). \quad (23) \]

Equations (21) and (22) will be rewritten further as follows:
\[ k_\infty(t) = \sum_j n_j(t) \nu_j A_j \sigma_{F,j} \] \[ \phi(t) = \frac{\nu_p(t)}{\sum_j n_j(t) \sigma_{F,j}}. \] (24)

Here we should be careful at the denominator of equation (24), neutron absorption term. The suffix \( j \) covers all of the nuclides in the core. However, in other parts \( j \) covers only nuclides produced in the core from the fuel, which are actinides and FPs. Now we define h-value as follows:

\[ h(t) = \frac{\sum_{j \in \text{FP}} n_j(t) \nu_j A_j \sigma_{F,j}}{\sum_{j} n_j(t) \sigma_{A,j}}. \] (26)

And h-value without FP as follows:

\[ h_{\text{Act}}(t) = \frac{\sum_{j \in \text{Act}} n_j(t) \nu_j A_j \sigma_{F,j}}{\sum_{j \in \text{Act}} n_j(t) \sigma_{A,j}}. \] (27)

Apparently the following equation holds:

\[ h_{\text{Act}}(t) > h(t) > k_\infty(t). \] (28)

Now we have delivered all necessary equations for our study, equations (23), (24) and (25). These equations consist the governing equations together with the equations for temperature and material distribution.

3. Fuel Burning Equation at Continuous Operation

3.1. Fuel burning equation at continuous operation

In the following parts equation (23) will appear often, and then we will rewrite it by using slightly different notations for convenience as follows:

\[ \frac{dn_j}{dt} = -(\lambda_j + \sigma_{A,j} \phi)n_j + \sum_k (\alpha_{k \rightarrow j} \lambda_k + \beta_{k \rightarrow j} \sigma_{A,k} \phi + \gamma_{k \rightarrow j} \sigma_{F,k} \phi)n_k. \] (29)

where

\( \lambda_j \): decay constant of nuclide \( j \),

\( \sigma_{A,j} \): microscopic absorption cross-section of nuclide \( j \),

\( \sigma_{F,j} \): microscopic fission cross-section of nuclide \( j \),

\( \alpha_{k \rightarrow j} \): branching ratio of decay of nuclide \( k \) to nuclide \( j \),
$\beta_{k \to j}$: branching ratio of neutron absorption of nuclide $k$ to nuclide $j$,
$\gamma_{k \to j}$: branching ratio of fission of nuclide $k$ to nuclide $j$.

Equation (26) does not include fuel managements. We need it for solving this equation. Here we study on continuous operation, where fuel charge and discharge are continuous. In this case we can treat the problem simply by adding charge and discharge terms into equation (26) as follows:

$$\frac{dn_j}{dt} = - (\lambda_j + \sigma_{A,j} \phi + r_j) n_j + \sum_k \left( \alpha_{k \to j} \lambda_k + \beta_{k \to j} \sigma_{A,k} \phi + \gamma_{k \to j} \sigma_{F,k} \phi \right) n_k + s_j,$$

where

$r_j$: discharge constant of nuclide $j$,
$s_j$: charge rate of nuclide $j$.

This equation can be written in a matrix form as follows:

$$\frac{dn}{dt} = - Mn + s,$$

where

$M$: transmutation matrix,
$n$: nuclide densities of actinides and FPs,
$s$: fuel supply rate.

The matrix $M$ and vector $n$ can be written as

$$M = \begin{bmatrix} M_{Act,Act} & 0 \\ -M_{Act,FP} & M_{FP,FP} \end{bmatrix},$$

$$n = \begin{bmatrix} n_{Act} \\ n_{FP} \end{bmatrix}.$$  \hfill (32)

$$n = \begin{bmatrix} n_{Act} \\ n_{FP} \end{bmatrix}.$$  \hfill (33)

Where suffixes Act and FP represent actinide and FP, respectively, and equation (31) can be decomposed as

$$\frac{dn_{Act}}{dt} = - M_{Act,Act} n_{Act} + s_{Act},$$

$$\frac{dn_{FP}}{dt} = M_{Act,FP} n_{Act} - M_{FP,FP} n_{FP} + s_{FP}.$$  \hfill (34)

From these equations we can see that the actinide density, $n_{Act}$, can be obtained without any information about FPs, and $h_{Act}$-value can be obtained by solving only equation (34).

The conventional reactor operation is batch operation, where the fuel charge and discharge operations are performed during the reactor shutdown period. In this reactor operation scheme $s = 0$ during the reactor operation period, and (31) can be solved as
\[ n = e^{-MT}n_B, \]  
\[ (36) \]

where \( n_B \) is the nuclide density vector at the beginning of cycle (BOC). For the cycle length of \( T \), the nuclide density vector at the end of cycle (EOC) \( n_E \) is given by

\[ n_E = e^{-MT}n_B. \]  
\[ (37) \]

If \( q \) is charged and \( d \) is discharged during the shutdown period, \( n_B \) can be given by the following equation:

\[ n_B = n_E + q - d. \]  
\[ (38) \]

By substituting Eq. (38) into equation (37)

\[ n_E = e^{-MT}(n_E + q - d). \]

Then

\[ (e^{MT} - I)n_E = (q - d)/T. \]

When \( \|MT\| \ll 1 \)

\[ Mn_E = (q - d)/T. \]  
\[ (39) \]

Usually we treat the set of equations (34) and (35) instead of equation (31).

We can rewrite \( h \) and \( h_{\text{Act}} \) by using vector notations as follows:

\[ h = \frac{\nu\sigma_f, n_{\text{Act}}}{\sigma_a, n}, \]  
\[ (40) \]

\[ h_{\text{Act}} = \frac{\nu\sigma_f, n_{\text{Act}}}{\sigma_a, n_{\text{Act}}}. \]  
\[ (41) \]

3.2. Nuclear equilibrium state

From the finiteness of the earth our society ultimately should become a steady state society where the energy consumption rate is a constant \([3]\). If this energy supply is satisfied by the fission energy, the fresh fuel charge rate and waste discharge rate are also constants. Furthermore, the reaction rate of each nuclear reaction and abundance ratio of each nuclide in the reactor are also constants \([4]\). This kind of state is called as the nuclear equilibrium state.

I call the society in this state the nuclear equilibrium society and continues to work under this research title for long period. In this society the energy production system is considered to affect the social system strongly. It is interested to know what kind of society will be realized as such a future society. However, we have many scientific and engineering problems to be investigated before studying the society itself.
We consider a nuclear energy center as shown in figure 1, in which several nuclear reactors and handling and storage facilities of nuclear fuels and wastes are operated. In the present scenario any radioactive materials will not be taken out of the nuclear energy center. Although we can consider many kinds of the nuclear equilibrium systems, we will study on simple systems at the beginning. The number of types of reactor is fixed to be one in order to know the fundamental effects of the reactor to the system, though the system with several kinds of reactors are possible and may work as an efficient synergetic system. The number of type of fuel is also chosen to be one, natural uranium or thorium.

![Figure 1. A simple model of nuclear equilibrium system](image)

In the present model, the natural uranium or thorium are supplied to the reactor in the center as shown in figure 1. All the actinides (including the daughter nuclides in the secular equilibrium with this nuclide) are confined in the reactor. Almost all of them will fission and only small amount becomes the terminal nuclides after radioactive decays; $^{204}$Pb, $^{206}$Pb, $^{207}$Pb, $^{208}$Pb and $^{209}$Bi. In this system these terminal nuclides of actinide decay chain and FPs are withdrawn from the reactor. Otherwise they are accumulated in the reactor.

3.3. Nuclear equilibrium equation

The nuclide composition in the reactor does not change along time for the nuclear equilibrium state. The rigid nuclear equilibrium state is investigated for the continuous operation as the simplest case. It may be a good approximation even for the batch-wise discontinuous fuel-cycle operation, and useful for the investigation of change of the state characteristics for different neutron spectra and inserted fuel.

Now we consider a region of unit volume in the reactor. Fuel is considered to be charged to this region with a constant rate. The nuclide that does not relate to the natural uranium or thorium is not considered in this analysis. The nuclides are transmuted in the reactor to other nuclides. The transmutation is performed with a nuclear reaction with a neutron and natural decays. Through these transmutations many kinds of nuclides present in the reactor in the equilibrium state.

The strict equilibrium nuclear state is a steady state, where the nuclide number density of each nuclide does not change, and the following equation holds:

$$\frac{dn}{dt} = 0.$$  \hspace{1cm} (42)

Therefore, Eq. (31) becomes
\( Mn = s \).  

(43)

or equations (34) and (35) become

\[
M_{Act,Act} n_{Act} = s_{Act},
\]

(44)

\[
M_{FP,FP} n_{FP} - M_{Act,FP} n_{Act} + s_{FP}.
\]

(45)

This equation is called as the nuclear equilibrium equation.

It is noted that the nuclear equilibrium equation (43) is similar to equation (39) which holds for \( \|MT\| \ll 1 \).

The nuclear equilibrium equation is a linear algebraic equation, and can be easily solved for constant coefficients. Many of these coefficients are the one-group constants defined by equations (18) through (20), which are neutron spectrum weighted values. When the neutron spectrum is given, these coefficients are constants and the nuclear equilibrium equation can be solved very easily. However, neutron spectrum changes for different nuclide density configurations. In such a case, \( M \) depends on \( n \) and we need a coupling code system of neutron spectrum calculation and nuclear equilibrium calculation. One of such a code system is shown in figure 2 [5].

![Equilibrium Cell Iterative Calculation System (ECICS) [5]](https://example.com/figure2)

3.4. Solution for Some Simple Problems [4]

Here we will solve equation (43) and obtain h-value by using equation (40) for a simple problem in order to investigate the possibility to realize a typical nuclear equilibrium state [4].

3.4.1. Calculation Conditions

Equation (43) is so simple that we can treat many nuclides without any calculation problems. All actinides whose half-life is more than one day are employed in the present analysis. Then 129 actinides and 1238 FPs are treated in the present study. In usual cases, however, much less number of nuclides is enough for evaluating neutron economy in an acceptable accuracy.
As typical reactors two types of fast reactors and two types of thermal reactors are investigated. For the fast reactors a sodium-cooled oxide-fuel fast reactor (soft fast) and a sodium-cooled metallic fuel fast reactor (hard fast) are treated, and for the thermal reactors a PWR (hard thermal) and a high moderation-ratio graphite-moderated gas-cooled reactor (soft thermal) are treated. The neutron spectra of these reactors are shown in figure 3.

![Diagram of neutron spectra](image)

**Figure 3.** Typical neutron spectra

The one-group constants are obtained by using these spectra and equations (18) thorough (20). Fundamental design parameters of the reactors are shown in table 1. The removal half-life is given by $T_{1/2} = \ln 2 / r$, where $r$ is the discharge constant (See equation (30)). These parameters are enough for the present stage of the study, since only general aspects are interested in.

**Table 1.** Fundamental reactor design parameters
3.4.2. Nuclide Densities
The obtained nuclide densities of all actinides more than $10^{15}/\text{cm}^3$ in a reactor charged with natural uranium or thorium are shown in figure 4 for soft fast or hard thermal reactors. Though in these figures only the cases for soft fast and hard thermal reactors are shown, the differences between hard fast and soft fast and between hard thermal and soft thermal are much smaller than the differences between fast and thermal.

The actinide nuclide number densities do not depend on the FP discharge constant, since they are obtained by solving (44) which does not include the FP discharge constant.

Apparently the densities of higher actinides are higher for the natural-uranium charge case than the thorium charge case and vice versa. The densities of charged nuclides are about the same for all four cases. The decrease amount from the charged nuclide to the next nuclide is larger for the thermal reactors than the fast reactors but the decreasing slope becomes slower.

|                     | Thermal Reactor | Fast Reactor |
|---------------------|-----------------|--------------|
| Total Power Output  | 3 GWt           | 3 GWt        |
| Power Density       | 50 W/cc         | 300 W/cc     |
| Removal Half Life   | 1 year          | 1 year       |
Figure 4. Equilibrium nuclide densities for different nuclear systems [5]
From these nuclide densities we can obtained many characteristics of each system. In the next section we will discuss the criticality. Discharged fuel characteristics are also easily evaluated by using these nuclide densities. However these topics are omitted from the page limit. I hope the readers who are interested in these topics will see some of the references [6, 7].

3.4.3. Criticality

The \( h \)-values obtained using the previously shown nuclide densities are shown in figure 5 for the FP removal half-life of 1 year, where the power density level is changed to investigate its effect. The horizontal axis denotes the neutron flux level which is proportional to the power density level. The flux level change causes change of the ratio of the neutron induced reaction to radioactive decay. Therefore, the nuclide density distribution along mass number will change, and \( h \)-value changes. For the thorium cycle case, \( h \)-value decreases with increasing flux level. It is attributed to the increasing neutron absorption by \(^{233}\text{Pa}\) for increasing flux level.
When we consider the neutron economy, 5 - 10% of produced neutrons are usually absorbed by construction materials, coolant, moderator, control materials, etc., and leakage from the system, though this amount depends strongly on the reactor design. Therefore, the h-value should take a value more than 1.03 - 1.1 to perform the criticality. Judging from these calculation results, the fast reactor charged with natural uranium can perform the criticality with some surplus, but the thermal reactor charged with natural uranium cannot perform it. The system with thorium may perform the criticality for both fast and thermal neutron system for lower neutron flux level, but it seems not easy. The fast reactor system shows the better performance also for this system, but the difference is small. The system showing the best neutron economy is the fast reactor system charged with natural uranium.

4. Nuclide Importances [8]

4.1. Importance and adjoint function

At the beginning on this chapter I will mention about some basic theory of linear systems. We start the discussion with the following linear state equation (governing equation)

\[ M|n\rangle = |s\rangle. \]  \hspace{1cm} (46)

This equation is a simple rewriting of equation (43) by using bra-vector and ket-vector, which are the notations introduced by Dirac for describing quantum mechanics [9], but convenient for describing our equations. The ket-vector \( |n\rangle \) is called the state vector, and \( |s\rangle \) is called the source vector. We consider an objective value (performance index) which is given by a scalar product of the source vector and the weight vector \( \langle w|n\rangle \) as follows:

\[ Q = \langle w|n\rangle. \]  \hspace{1cm} (47)

If this objective value can be written as
\[ Q = \langle i | s \rangle. \]  

(48)

The bra-vector \( \langle i | \) is called an importance vector, or \( i_j \) is called an importance of \( s_j \).

From equations (46) through (48)

\[ \langle w | n \rangle = Q = \langle i | s \rangle = \langle i | M | n \rangle. \]

Therefore

\[ \langle i | M = \langle w |. \]

(49)

This is the adjoint equation to equation (46), where the adjoint source is the weight vector. We see the importance vector is the adjoint vector.

Equations (44) and (45) can be rewritten by the present way

\[ M_{\text{Act,Act}}|n_{\text{Act}}\rangle = |s_{\text{Act}}\rangle, \]

(50)

\[ M_{\text{FP,FP}}|n_{\text{FP}}\rangle = M_{\text{Act,FP}}|n_{\text{Act}}\rangle + |s_{\text{FP}}\rangle. \]

(51)

The equations corresponding to equations (47) and (48) are as follows:

\[ Q = \langle w_{\text{Act}} | n_{\text{Act}} \rangle + \langle w_{\text{FP}} | n_{\text{FP}} \rangle, \]

(52)

\[ Q = \langle i_{\text{Act}} | s_{\text{Act}} \rangle + \langle i_{\text{FP}} | s_{\text{FP}} \rangle. \]

(53)

And the adjoint equations are as follows:

\[ \langle i_{\text{Act}} | M_{\text{Act,Act}} = \langle i_{\text{FP}} | M_{\text{Act,FP}} + \langle w_{\text{Act}} |. \]

(54)

\[ \langle i_{\text{FP}} | M_{\text{FP,FP}} = \langle w_{\text{FP}} |. \]

(55)

4.2. Examples of importance

Some examples of weight (adjoint source) and corresponding importance are shown in table 2.
Table 2. Adjoint sources, $w_j$, for several importances, $i_j$, of nuclide $j$ [8]

| Importance                                      | $i_j$                           | $w_j$                           |
|------------------------------------------------|---------------------------------|---------------------------------|
| Nuclide number importance (total number of nuclides) | $i_{n,j}$                       | 1                               |
| Fission number importance (total number of fissions) | $i_{f,j}$                       | $\phi \sigma_{f,j}$            |
| Fission neutron importance (total number of produced fission neutrons) | $i_{\nu f,j}$                  | $\phi \nu \sigma_{f,j}$        |
| Absorbed neutron importance (total number of absorbed neutrons modified by neutron producing reactions except fission) | $i_{a,j}$                       | $\phi \left( \sigma_j - \sum m \sigma_{m,j} \right)$ |
| Net neutron production importance (net number of produced neutrons) | $i_{p,j}$                       | $\phi \left( \nu \sigma_{f,j} - \sigma_j + \sum m \sigma_{m,j} \right)$ |

In this section some calculated values of importances are presented for the systems shown in section 3.4, but the neutron spectra of fission neutron, soft fast reactor (fast reactor), hard thermal reactor (thermal reactor) and thermal Maxwellian spectrum are used to obtain one-group cross sections for studying the difference of neutron spectrum.

The first example is the fission number importance, which is shown in table 3. The importances of important actinides are almost unity for reactor spectra. It means that almost all important actinides will ultimately fission for these conditions. Where the neutron energy becomes higher, the number of nuclides produced by $(n, 2n)$ reaction of light actinide increases, and the some small part of produced nuclides escape fission and decay more easily to lighter nuclides finally to a stable isotope such as $^{204}$Pb, $^{206}$Pb, $^{207}$Pb, $^{208}$Pb and $^{209}$Bi as mentioned in section 3.2. And then the fission number importance decreases from unity by a small amount. The lower neutron flux level makes the importance decrease, since the ratio of fission reaction to radioactive decay decreases.

The next example is the net neutron importance, which is shown in figure 6. The results in this figure are for the case of FP discharge constant of infinity and 1/2 $\gamma^{-1}$ and for the case of neutron flux level of $10^{15}$ cm$^{-2}$s$^{-1}$. The importance generally increases with increasing mass number. This behavior is monotonic for the fission neutron spectra, but it is oscillatory for the reactor spectra. For the change of discharge constant from infinity to 1/2 $\gamma^{-1}$, the importance shifts downward. This tendency is especially dominant for the softer spectrum. For the fast reactor, the importances of almost all actinides are positive for all cases, but the $^{238}$U importance is negative. The negativeness becomes more severe for the thermal reactor. Then for the thermal reactor the multi-recycle of uranium makes neutron economy considerably worse.

More importances and more detail discussions on these results are given in reference [8].
Table 3. Fission number importance [8]

| Neutron Spectrum | fission | fast reactor | thermal reactor | Maxwellian |
|------------------|---------|--------------|-----------------|------------|
|                  | $10^{15}$ | $10^{16}$     | $4.72 \times 10^{15}$ | $2.17 \times 10^{16}$ | $10^{15}$ | $10^{16}$ |
| Th-232           | 0.99726  | 0.99972      | 0.99994         | 0.99989     | 1.00000   | 1.00000   |
| U-233            | 0.99974  | 0.99997      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| U-234            | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| U-235            | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| U-236            | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| U-238            | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Np-237           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Pu-238           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Pu-239           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Pu-240           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Pu-241           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Pu-242           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Am-241           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Am-242m          | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Am-243           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Cm-243           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Cm-244           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Cm-245           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Cm-246           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Cm-247           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |
| Cm-248           | 1.00000  | 1.00000      | 1.00000         | 1.00000     | 1.00000   | 1.00000   |

Figure 6. Net neutron importance ($\phi = 10^{15} \text{cm}^{-2}\text{s}^{-1}$) [8]
4.3. Criticality search for continuous operation

Generally criticality search is complicated and difficult to be performed. Even the simple system given in chapter 3 may take a lot of time for criticality search by adjusting flesh fuel compositions. If we employ the nuclide importances, it becomes a simple and easy procedure [10]. Here we try to find the charged fuel compositions to make a system critical for equilibrium cycle.

For the criticality condition, \( k_{\text{eff}} = 1 \), we consider that \( h \)-value takes the value \( h_c \), where

\[
h_c > 1.
\]  \( (56) \)

If we have an acceptably accurate value of \( h_c \), we can obtain the proper source term \( |s| \) to give the criticality by solving the following equation:

\[
\langle i_{\nu} - h_c i_a | s \rangle = 0,
\]  \( (57) \)

where the importances \( \langle i_{\nu} \rangle \) and \( \langle i_a \rangle \) are obtained from the following equations:

\[
\langle i_{\nu} \rangle M = \langle \phi \nu \sigma_{\nu} \rangle ,
\]  \( (58) \)

\[
\langle i_a \rangle M = \langle \phi \left( \sigma - \sum_{m} m \sigma_{m} \right) \rangle .
\]  \( (59) \)

We will show some examples for demonstration of this methods, where the reactor is a PWR and its design parameters are shown in table 4 [10].

| Table 4. Design parameters of studied PWR |
|------------------------------------------|
| Power Output (MW thermal)                | 3000 |
| Average power density of Pellet (Wcm\(^{-3}\)) | 280  |
| Average power density of Cell (Wcm\(^{-3}\)) | 100  |
| Fuel Pellet diameter (mm)                | 8    |
| Pin diameter (mm)                        | 9.6  |
| Pin pitch (mm)                           | 11.8 |
| Materials                                |      |
| Fuel pellet                              | Oxide|
| Cladding                                 | Zircaloy 4|
| Coolant                                  | Light water|
| Volume fraction (%)                      |      |
| Fuel pellet                              | 36   |
| Cladding                                 | 16   |
| Coolant                                  | 48   |

We apply five in-core fuel management cases as shown in table 5, and try to find the enrichment and some other reactor characteristics for each scheme. The discharge constant for the standard operation is chosen as \( 1/3 \) yr\(^{-1}\), in order to simulate in-core fuel management for three batches. The calculation system like figure 2 should be employed, since the neutron spectrum changes for different cases, and
the changes of parasitic absorptions by non-fuel materials (construction materials and water) and leakage should be also evaluated. The details of this procedure are written in reference [10].

Table 5. Discharge constant for 5 in-core fuel managements ($r = 1/3 \text{ yr}^{-1}$)

| Case | U | Pu | Other Actinides |
|------|---|----|----------------|
| 1    | r | r  | r             |
| 2    | r | $r/2$ | r      |
| 3    | r | 0  | r             |
| 4    | r | 0  | 0             |
| 5    | 0 | 0  | 0             |

The obtained results are shown in table 6. The obtained results represent well the characteristics of once-through and recycle systems, which are discussed widely in nuclear energy society. The plutonium and minor actinides recycle can reduce the required natural uranium amount as expected, but their effects are not so large. If the enrichment is increased enough, we can burnup whole charged fuel and reduce the required natural uranium amount considerably. However, the value of enrichment becomes higher than 20 % which cannot be permitted for commercial uses, and the burnup of discharged fuel is too much for satisfying the material constraints.

Table 6. Required enrichment and several fuel cycle characteristics [10]

| Case | $h_c$ | Enrichment ($\%$) | Charged fuel (t/y) | Flux ($\text{cm}^{-2} \cdot \text{s}^{-1}$) | Burnup (GWd/t) | Required Natural U (t/y) |
|------|------|-----------------|------------------|-----------------|----------------|-------------------------|
| 1    | 1.046 | 4.2             | 29               | $3.83 \times 10^{14}$ | 37.9          | 195.4 276.3 |
| 2    | 1.041 | 4               | 28.8             | $3.80 \times 10^{14}$ | 38.1          | 185.3 261.4 |
| 3    | 1.031 | 3.8             | 28.1             | $3.73 \times 10^{14}$ | 39            | 169.2 237.9 |
| 4    | 1.030 | 3.6             | 27.6             | $3.71 \times 10^{14}$ | 39.8          | 158.9 222.8 |
| 5    | 1.026 | 41.6            | 1.2              | $3.46 \times 10^{14}$ | 952.7         | 79.4 117.5 |

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