86. Calculation of the Effective Thermal Cross-section and Its Temperature Coefficient, (I)

The effective thermal cross-section

By Akinao SHIMIZU*

An approximate expression for the effective thermal cross-section of an element in the infinite homogeneous medium with $1/\nu$ absorption is derived from the monoatomic heavy gas model with the aid of the variational principle. Comparison with the exact numerical value shows that the error due to the derived approximate expression is less than several percent in the range, $0 \leq \Sigma a(kT)/E \Sigma \delta a \leq 1.0$. An approximate expression for the epithermal reaction which is consistent with the derived one for the thermal reaction is also presented.

INTRODUCTION

In the calculation of the effective reaction in the thermal region, two kinds of methods are currently used. According to the first method, a neutron thermal spectrum is assumed to be the Maxwellian distribution corresponding to a neutron temperature, which joins $1/E$ distribution at an appropriate energy. Although this intuitive picture of the thermal spectrum leads to a tractable expression of the effective cross-section, its validity is obscure and the applicability is limited to a well-moderated reactor where

$$\Sigma a(kT)/E \Sigma \delta a \leq 0.1 \text{ (or 0.2)}$$

The other method is a numerical calculation based on a suitable thermalization model with the aid of a digital computer. The physical basis is obtained by this method at a sacrifice of an intuitive expression of the effective cross-section, as far as an applied model is adequate.

The purpose of the present article is to derive a simple expression of the effective cross-section applicable to a wider range of $\Sigma a(kT)/E \Sigma \delta a$ from a thermalization model. In the Cap. I the thermalization model applied to the present calculation is described. In the Cap. II, a variational expression for the effective cross-section\(^{(1)}\) is described, and the effective thermal cross-section is expressed by a simple formula. In the Cap. III, the accuracy of the derived formula is examined by comparison with numerical solutions of the thermalization equation. In the Cap. IV, an approximate form of an epithermal spectrum is derived.

I. THERMALIZATION MODEL

The present calculation of the effective thermal cross-section is carried out under the following assumptions.

(1) The energy interval from zero to the cut-off energy $E_m$ is defined as the thermal region and the reaction in the thermal region is treated separately from that in the epithermal region. The cut-off energy $E_m$ is such that in the region $E > E_m$, the effect of the thermal motion on the neutron spectrum is small and the neutron spectrum is almost $1/E$ distribution. In the present calculation, $E_m$ is selected as $10kT$, where $T$ is the temperature of the medium.

The effective thermal cross-section $\delta_{th}$ is defined by an equation.

$$\delta_{th} = \int_0^{E_m} \sigma(E)\Phi(E)\,dE / \int_0^{E_m} E\Phi(E)\,dE$$

\(^{(1)}\)
where $\Phi(E)$ is the neutron flux per unit energy interval and $E_0 = 0.0253$ eV.

(2) The medium is assumed to be infinite and homogeneous. We further assume that the main absorption of the medium is $1/\nu$ absorption.

(3) The relation between the neutron flux and the slowing down density is assumed to be expressed by an equation

$$q(E) = \xi \sum (E-kT_0) \Phi(E) + kT \cdot E \frac{d\Phi}{dE}$$

which is derived from the monoatomic heavy gas model, in the thermal region and in the epithermal region near the energy $E_m$. $\xi \sum$ is the slowing down power of free atoms and is assumed to be independent of energy. The source term is included as the boundary condition that $\Phi(E_m)$ should be equal to the given value. The relation (2) and the number balance equation,

$$\frac{dq}{dE} = \sum_{a} (E) \Phi(E)$$

where $\sum_a (E)$ is an absorption cross-section of the medium which is assumed to be under $1/\nu$ law, lead to a differential equation for the flux, so called “Wilkins equation”. A normalized solution of this equation, $\Phi(E)/\phi_{\text{th}}$, where

$$\phi_{\text{th}} = \int_{E_0}^{E_{\text{max}}} \sqrt{\frac{E}{E_0}} \Phi(E) dE$$

is determined uniquely by the boundary condition at zero energy,

$$q(0) = 0$$

$[\Phi(E)/M(E)]_{E=0}$ is finite

where $M(E)$ is the Maxwellian distribution. This spectrum depends upon two parameters, $\sum_a(kT)/\xi \sum$, and the temperature of the medium, $T$. However, changing the variable $E$ to $E/kT$ the parameter $T$ disappears and the form of the spectrum becomes dependent on only one parameter, $\sum_a(kT)/\xi \sum$, which we call $\Delta$, although the parameter $\Delta$ currently used is the abbreviation of $4 \sum_a(kT)/\xi \sum$.

II. VARIATIONAL FORMULATION

In terms of new variables,

$$\tilde{E} = \frac{E}{kT}, \quad \tilde{\Phi}(E) = \Phi(E)/M(E), \quad M(E) = \epsilon e^{-\epsilon}$$

Eqs. (2) and (3) can be rewritten as

$$q(\tilde{E}) = \xi \sum M(\tilde{E}) \epsilon \frac{d\Phi}{d\tilde{E}}$$

where

$$\frac{d\Phi}{d\tilde{E}} = \sum_a (\tilde{E}, kT) \Phi(\tilde{E})$$

which is derived from the monoatomic heavy gas model, in the thermal region and in the epithermal region near the energy $E_m$. $\xi \sum$ is the slowing down power of free atoms and is assumed to be independent of energy. The source term is included as the boundary condition that $\Phi(E_m)$ should be equal to the given value. The relation (2) and the number balance equation,

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This type of solution gives a more rigorous and simpler expression of the effective thermal cross-section than the crude spectrum, the Maxwellian distribution with the neutron temperature plus $1/E$ distribution, but its applicability is limited for small $\Delta$. However, with the aid of a suitable functional of $\Psi$, which is an extremum for $\Phi$ satisfying Eqs. (5) and (6) and the extremum of which is the desired effective thermal cross-section, and a trial function

$$\Psi = 1 + \beta Q(\epsilon)$$

one obtains the expression of the effective thermal cross-section which is simple and accurate for the wider range of $\Delta$.

Assuming that the absorption cross-section of the desired element, $\sigma(E)$ is expressed as

$$\sigma(E) = \sigma_0 \sqrt{\frac{E_0}{E}} f(E)$$

where $\sigma_0 = \sigma(E_0)$ and $f(E)$ represents the non $1/\nu$ character of $\sigma(E)$, the following functional of $\Psi$ and an auxiliary function $\chi$ is proved to have the above mentioned property,

$$J(\Psi, \chi) = \int_{E_0}^{E_m} \left[ \chi \sum_\epsilon M(\epsilon) \chi d\epsilon \right] + \int_{E_0}^{E_m} \sum_\epsilon M(\epsilon) \chi d\epsilon$$

where

$$\sum_\epsilon M(\epsilon) = \sum_\epsilon \sum \epsilon M(\epsilon) \chi$$

The functional is stationary for $\Psi$ satisfying Eqs. (5) and (6) and for $\chi$ satisfying an equation

$$\frac{d\chi}{dE} = \sum_\epsilon \epsilon M(\epsilon) \frac{d\Phi}{dE}$$

where

$$\sum_\epsilon \epsilon M(\epsilon) \frac{d\Phi}{dE} = \sum_\epsilon \epsilon M(\epsilon) \frac{d\Phi}{dE}$$

For small $\Delta$, the iterative solution of Eqs. (5) and (6),

$$\Psi(\epsilon) = 1 + \Delta \cdot Q(\epsilon) + O(\Delta^2)$$

$$Q(\epsilon) = \int_0^\infty dZ Z^{-1} \epsilon^2 \int_0^\infty d\nu \epsilon e^{-\epsilon}$$

is derived by Hurwitz, et al.
\[
\frac{d}{de} \left\{ \xi \sum \frac{\partial}{\partial \varepsilon} \frac{\partial}{\partial \varepsilon} \chi \right\} - \sum \phi(\varepsilon) M(\varepsilon) X = 0 \tag{10}
\]

where \( \lambda = \frac{\sum M(\varepsilon)}{\int M(\varepsilon) d\varepsilon} \)

and the stationary value becomes

\[
J(\Psi, \chi) = \int_0^{\epsilon_m} \sum \phi d\varepsilon = \frac{\delta_{th}}{\sigma_0} \tag{11}
\]

In order to calculate \( J(\Psi, \chi) \) one should estimate the form of \( \chi(\varepsilon) \) as well as that of \( \psi \). Eq. (10) shows that \( M(\varepsilon) \) can be interpreted as a neutron spectrum under the external source

\[
S(\varepsilon) = \lambda \sum M(\varepsilon) \cdot M.
\]

In the case that \( f(E) \) is independent of \( E \), the solution of Eq. (10) becomes

\[
\chi = 1.
\]

Estimation of the form of \( \chi \) in the general case is difficult. However we may expect that the departure of \( \chi \) from unity is smaller than that of \( \psi \).

In the present calculation we select the form of \( \chi \) as

\[
\chi = 1 + \alpha \cdot \varepsilon
\]

\[\alpha: \text{a variational parameter}\]

although its adequacy is obscure.

The trial functions

\[
\chi = 1 + \alpha \cdot \varepsilon
\]

\[
\psi = 1 + \beta \cdot Q(\varepsilon)
\]

and the functional (9) lead to the expression,

\[
\frac{\delta_{th}}{\sigma_0} = \frac{\varepsilon_m(T) + \varepsilon_m(T) \cdot \Delta}{1 + 0.4300 \cdot \Delta} \tag{12}
\]

where \( T \) is the temperature of the medium

\[
\Delta = \frac{\sum \phi(\varepsilon)}{\sum \phi(\varepsilon)} \cdot M(\varepsilon) d\varepsilon
\]

\[
\varepsilon_m = 1.2857 \int \varepsilon \phi d\varepsilon
\]

\[
\varepsilon_m = 0.3494 \int \varepsilon \phi d\varepsilon
\]

\( \varepsilon_m = 10 \).

III. ACCURACY OF THE FORMULA

In order to examine the accuracy of the derived formula (12), comparison of the result by the formula (12) with the exact one obtained by a numerical calculation is made for the simple case that \( f(E) \) is expressed by an equation,

\[
\frac{\sqrt{E}}{\sqrt{E_0}} \sigma(E) \equiv f(E) = \gamma_0 + \gamma_1 \cdot E + \gamma_2 \cdot E^2 + \gamma_3 \cdot E^3 \tag{13}
\]

where \( \gamma_0, \gamma_1 \) are arbitrary constants.

In this case, \( \delta_{th} \) can be written as

\[
\frac{\delta_{th}}{\sigma_0} = \gamma_0 + \gamma_1 \cdot E + \gamma_2 \cdot E^2 + \gamma_3 \cdot E^3
\]

where \( \langle E^m \rangle \) is the mean value of \( E^m \) of thermal neutron and expressed as

\[
\langle E^m \rangle = \frac{\int_0^{\epsilon_m} \frac{1}{\sqrt{E}} \phi(E) dE}{\int_0^{\epsilon_m} \frac{1}{\sqrt{E}} \phi(E) dE} = \langle (kT)^m \rangle
\]

\[
\langle E^m \rangle = \frac{\int_0^{\epsilon_m} \frac{1}{\sqrt{E}} \phi(E) dE}{\int_0^{\epsilon_m} \frac{1}{\sqrt{E}} \phi(E) dE} = \langle E^m \rangle
\]

\[
\delta_{th} = \frac{\gamma_0 + \gamma_1 \cdot E + \gamma_2 \cdot E^2 + \gamma_3 \cdot E^3}{1 + 0.4300 \cdot \Delta}
\]

The values of \( \langle E^m \rangle \) according to Eq. (14) are compared with the exact value obtained by the numerical calculation, the detail of which is described in the Appendix B. The results are presented in Table 1, which shows that the effective thermal cross-section can be estimated by the formula (12) with an error less than 7% in the range of \( 0 \leq \Delta \leq 1.0 \), as far as \( \sigma(E) \) is expressed by Eq. (13).

If \( \gamma_0 \) in Eq. (13) which represents the contribution of the term independent of the spectrum to the effective thermal cross-section is large, the error becomes much less than 7%. As the absorption and fission cross-sections of major elements are approximately expressed by the Eq. (10) with an accuracy sufficient for the estimation of the order of the error due to the formula (12), we may conclude that the validity of the effective cross-section calculated by the formula (12) is almost equivalent to that of the aforesaid thermalization model in the range of \( 0 \leq \Delta \leq 1.0 \).
of some elements which are calculated according to the formula (12) and Westcott's analytical fit of the curves of $f(E)$ to an equation of the form

$$f(E) = \frac{a(kT)}{f(E)}$$

are given.

### IV. EPITHERMAL REACTION

The ratio of the reaction in the thermal region to that in the epithermal region is obtainable if the spectrum $f(E)/f_\text{th}$ in the epithermal region is known. This epithermal spectrum is estimated as follows. One assumes that the relation

$$q(E) = \xi \sum_i \left( (E-kT)^i \Phi(E) + kTE \frac{d\Phi}{dE} \right)$$  \hspace{1cm} (15)

still holds in the epithermal region. With the aid of the fact that $E$ is much larger than $kT$ in this region, an approximate form of the epithermal spectrum is derived from the relation (15) and Eq. (3). Next this approximate spectrum is adjusted so that it may continue at $E_M$ to $f(E_M)/f_\text{th}$ which is determined by the balance equation in the thermal region.

1. The estimation of $\Phi(E_M-0)/\Phi_\text{th}$ from the balance equation in the thermal region

$\Phi(E_M-0)/\Phi_\text{th}$ is estimated by the following variational procedure. Consider the functional of $\Psi$

$$K(\Psi) = \int_0^\infty \frac{M(\xi) \Psi'(\xi)}{q(\xi)} d\xi$$  \hspace{1cm} (16)

It is an extremum for $\Psi$ satisfying Eqs. (5) and (6) and the extremum is

$$K(\Psi) = \frac{\phi(\xi)}{q(\xi)}$$

Furthermore, as $\xi \sum_i \xi M$ and $\sum_i M$ are both positive the inequality $K(\Psi_\text{tri.}) < K(\Psi)$ holds for any $\Psi_\text{tri.}$ satisfying the boundary condition (4). With the aid of a trial function,

$$\Psi_\text{tri.} = 1 + \beta \cdot Q(\xi)$$

$\beta$: variational parameter

we get for $\xi = 10$

$$\frac{\xi \sum_i \Phi(\xi)}{q(\xi)}$$

$$= \frac{M(\xi)(1 + 254.852 \Delta)}{\Delta \int_0^\infty \frac{1}{\xi} M(\xi) d\xi + 0.085886 \cdot \Delta}$$  \hspace{1cm} (17)

where $\int_0^\infty \frac{1}{\xi} M(\xi) d\xi = 0.88078$

The accuracy of the obtained formula is examined by comparison with the exact value. The result is presented in Table 2. It shows that the error is less than 2.5% for the range of $\Delta$, $0 \leq \Delta \leq 1.0$ and the sign of the error is minus as expected.

Eq. (17) and the relation

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<th>V.C</th>
<th>Exact</th>
<th>Error(%)</th>
<th>V.C</th>
<th>Exact</th>
<th>Error(%)</th>
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<th>Error(%)</th>
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Table 2 Accuracy of the formula (17)

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<th>Error(%)</th>
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</table>

\[ \xi \sum \phi(\xi) | q(\xi) \]

2. Derivation of an approximate expression of the epithermal spectrum

The relation (15) can be rewritten as

\[ q(E) = \xi \sum \phi(E) dE = \xi \sum a \phi_{th} \]

where

\[ \Delta = \frac{\sum \phi_{th}}{\xi \sum a} = \sqrt{\frac{T}{T_0}} \Delta \]

lead to the expression

\[ \frac{\phi(\xi_{th} = 0)}{\phi_{th}} = \sqrt{\frac{T}{T_0}} \frac{M(\xi)}{0.886078 + 0.055056 \cdot \Delta} \]

where

\[ M(\xi) = \frac{E_{th}}{kT} e^{-E_{th}/kT} \]

3. The effective cross-section and conversion factors

Let's define the effective cross-section, \( \sigma_{eff} \), as

\[ \sigma_{eff} = \int_{E_{th}}^{\xi_{th}} \frac{\sigma(E) \phi(E) dE}{\sqrt{E_{th} E}} \]

where

\[ \sigma_{eff} = \frac{\sigma_{th}}{\sigma_{0}} + \Delta \sigma_{\gamma} + a \cdot \delta_{x} \]

...
The last term in Eq. (24) is negligible except for special elements which have a high resonance level near the energy $E_M$. However this term becomes more important in the estimation of the temperature coefficient of the effective reaction rate.

$\sigma_v S_\alpha$ is the resonance integral including $1/d$ absorption down to $E_M$ with a correction due to the thermal motion of the moderator, which is important for elements which have high resonances near the energy $E_M$. When the medium contains many resonance absorbers such as $^{238}\text{U}$, the depression of the spectrum near the resonance levels should be taken into account.

As various definitions of the effective cross-section are used, a conversion factor of a definition to another was evaluated with the aforesaid thermalization model. Only the results are presented in the below.

\[
\int_{E_M}^{\infty} \sqrt{\frac{E}{E_M}} \Phi(E) dE = \sqrt{\frac{T_0}{T}} \left[ 1 + 0.4300 \cdot \Delta \right] + 1.1280 + 1.4464 \cdot \Delta
\]
\[
\int_{E_M}^{\infty} \frac{E}{E_M} \Phi(E) dE = \exp \left\{ \frac{2}{\sqrt{10}} \left( 1 + \frac{b}{30} \right) \Delta \right\}
\]
\[
+ 0.0001681 \frac{1}{1 + 0.09693 \cdot \Delta}.
\]

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(1) A. Shimizu: This Journal, 1, 376 (1959).

[APPENDIX A]

Table of $g_{th}$ and $s_{th}$

The values of $g_{th}$ and $s_{th}$ are calculated according to the formula (12). In these calculations the curves of $\sigma(E)$ are assumed to have the form

\[
\sqrt{E} \sigma(E) = a + \sum_{i=1}^{n} \frac{c_i}{(E - E_i)^2}
\]

the constants of which, $a$, $c_i$, $b_i$ and $E_i$ are reported by C. H. Westcott. The energy interval $0 \leq E \leq 10$ are divided into 500 meshes, and the value of $Q(E)$ at each mesh point is calculated by the same method as described in the Appendix B with the error less than $2 \times 10^{-5}$. Then the values of $g_{th}$ and $s_{th}$ are evaluated by the numerical integration according to the Sympon's formula.

<table>
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<tr>
<th>$T(\degree C)$</th>
<th>$^{239}\text{U}_{abs.}$</th>
<th>$^{231}\text{U}_{fission}$</th>
<th>$^{238}\text{P}_{abs.}$</th>
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APPENDIX B

Numerical Calculation of \( \langle \varepsilon^n \rangle \)

For the numerical calculation, it is convenient to change the variable \( \varepsilon \) in to \( x = \sqrt{\varepsilon} \). In terms of the new variable \( \langle \varepsilon^n \rangle \) is expressed with the equation,

\[
\langle \varepsilon^n \rangle = \int_{0}^{1} x^n \sqrt{\varepsilon} \phi(\varepsilon) d\varepsilon / \int_{0}^{1} \sqrt{\varepsilon} \phi(\varepsilon) d\varepsilon = \int_{0}^{1} x^n \sqrt{\varepsilon} \psi(x) dx / \int_{0}^{1} \sqrt{\varepsilon} \psi(x) dx
\]  

(1)

where \( \psi(x) \) is the solution of the equation

\[
x^2 \frac{d^2 \psi}{dx^2} + (3 - 2x^2) \frac{d\psi}{dx} - 4 \Delta \psi = 0
\]  

(2)

with the boundary condition

\[
x^3 e^{-x^2} \frac{d\psi}{dx} = 0 \quad \text{at} \quad x = 0
\]

\[
\psi(0) = 1.
\]

This solution can be expressed with the power series of \( x \),

\[
\psi(x) = \sum_{n=0}^{\infty} a_n x^n
\]  

(3)

\[
a_0 = 1, \quad a_1 = \frac{4}{3} \Delta,
\]

\[
a_{n+1} = \left[ \frac{4 \Delta a_n + 2n - 11a_{n-1}}{(n+1)(n+3)} \right].
\]

Now consider the function, \( f_n(y) \) defined as

\[
f_n(y) = \int_{0}^{y} x^{2(n+1)} e^{-x^2} \psi(x) dx.
\]

With the aid of Eq. (3) one gets the expression of \( f_n(y) \) with the power series of \( y \),

\[
f_n(y) = y^{2(n+1)} e^{-y^2} \sum_{n=1}^{\infty} b_n y^n
\]

\[
\begin{align*}
b_1 &= a_0 / (2(m+1)+1) \\
b_2 &= a_1 / (2(m+1)+2) \\
b_{n+1} &= (2b_{n-1} + a_n) / (2(m+1)+n+1)
\end{align*}
\]

and the desired \( \langle \varepsilon^n \rangle \) can be evaluated by an equation

\[
\langle \varepsilon^n \rangle = \frac{f_n(y)}{f_0(y)} \quad y = \sqrt{10}.
\]

In the numerical calculation the series \( \sum_{n=1}^{\infty} b_n y^n \) is approximated by \( \sum_{n=1}^{N} b_n y^n \). However it can be proved that for the given value of \( y \) and an arbitrary small positive constant, \( \delta \), there exists \( N \) which satisfies the inequality,

\[
\left| \frac{\sum_{n=1}^{\infty} b_n y^n - \sum_{n=1}^{N} b_n y^n}{\sum_{n=1}^{\infty} b_n y^n} \right| < \delta.
\]

In the present calculation \( \varepsilon \) is selected \( 2 \times 10^{-7} \) for \( y = \sqrt{10} \).

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熟中性子実効断面積とその
温度係数の計算, (I)

熟中性子実効断面積

清水 彰 直

重い単原子ガスモデルともついで、1/ν型吸収線
一様媒質中におかれた元素の熟中性子実効断面積の簡
単な近似表現を変分法を使って求められた。つぎに同
じモデルにもとづいた正確な値と比較した結果、得ら
れた近似式の誤差は \( 0 \leq \sum_{n=1}^{\infty} (kT) / \xi \leq 1.0 \) の範囲で、
大部の元素に対して数%以下であることが推定され
る。

また、熟外領域における反応の実効値の近似表現
も、同じモデルにもとづいて導かれた。