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Calculational Model for the Resonance
Absorption in the Pu²⁴⁰ 1 eV Resonance

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I. Introduction

This report presents a model for the inclusion of effects due to the thermal motion and chemical binding of protons on the resonance absorption in the Pu^{240} 1 ev resonance, in a lattice consisting of fuel rods in water. The model converts the heterogeneous problem of a rod in a lattice cell to a homogeneous problem. The procedure used here is essentially the same as the procedure used in the Multiple-Sauer method (Ref. 1); however, an independent derivation based on the Chernick coupled integral equations (Ref. 2) will be given. This derivation clarifies certain elements of the analysis, especially those concerned with whether a transport-corrected scattering cross section should be used in the water.

After converting the problem to an equivalent homogeneous problem, an approximation due to Cady and others (Ref. 3) is used for the hydrogen scattering kernel. The resonance absorption is then shown to be of the same form as that in HAMMER (Refs. 7,8) with a modified Dancoff factor in the

resonance integral computation and a modified value of the slowing down power $\xi \sigma_s$ for hydrogen. It is therefore easy to make the required changes to the HAMMER code.

II. Reduction of the Heterogeneous Problem to a Homogeneous Problem

We assume that scattering with respect to oxygen and all elements other than the hydrogen is heavy-element scattering and occurs without energy change. The modifications to the resonance integral which are obtained in this way will be assumed to apply to the resonance integral calculation in HAMMER, in which the effects of moderation of the oxygen in the fuel and the heavy elements is taken into account. The Chernick coupled integral equations for this system are

$$\begin{aligned} \Sigma_{Tf} V_f \bar{\phi}_f(E) = & V_m P_m^* \int \Sigma_{sm}(E \leftarrow E') \bar{\phi}_m(E') dE' \\ & + V_f (1 - P_f^*) \Sigma_{sf} \bar{\phi}_f(E) \end{aligned} \quad (1)$$

$$\begin{aligned} \Sigma_{Tm} V_m \bar{\phi}_m(E) = & V_m (1 - P_m^*) \int \Sigma_{sm}(E \leftarrow E') \bar{\phi}_m(E') dE' \\ & + V_f P_f^* \Sigma_{sf} \bar{\phi}_f(E) \end{aligned} \quad (2)$$

Here, P_f^* and P_m^* are first-flight lattice escape probabilities from the fuel and moderator regions, respectively. They are calculated on the basis of spatially flat isotropic source distributions in the fuel and moderator regions, respectively. In the limit when the resonance is narrow with respect to scattering by hydrogen, the hydrogen scattering cross section which should be used in calculating P_m^* should be the true hydrogen scattering cross section and not the transport-corrected cross section, since all scattering by hydrogen acts as removal from the resonance energy region, in the narrow-resonance limit. Hence, the transport correction will not be made in this analysis. In this respect, the calculation will differ from that of a THERMOS calculation.

The P_f^* and P_m^* obey the reciprocity relation:

$$\sum_{Tm} V_m P_m^* = \sum_{Tf} V_f P_f^* \quad (3)$$

Define $S(E)$ by

$$S(E) = \int_0^\infty \sum_{sm} (E+E') \bar{\phi}_m(E') dE' \quad (4)$$

Using Eqs. (3) and (4) in Eqs. (1) and (2), we obtain

$$\Sigma_{Tf} V_f \bar{\phi}_f(E) = \frac{\Sigma_{Tf}}{\Sigma_{Tm}} V_f P_f^* S(E) + V_f (1 - P_f^*) \Sigma_{sf} \bar{\phi}_f(E) \quad (5)$$

$$\Sigma_{Tm} V_m \bar{\phi}_m(E) = V_m \left(1 - \frac{\Sigma_{Tf} V_f}{\Sigma_{Tm} V_m} P_f^*\right) S(E) + V_f P_f^* \Sigma_{sf} \bar{\phi}_f(E) \quad (6)$$

The solution of Eqs. (5) and (6) is proportional to $S(E)$. If we denote by $\bar{\phi}_{fo}(E)$ and $\bar{\phi}_{mo}(E)$ the solution of Eqs. (5) and (6) with $S(E)$ replaced by unity, then

$$\begin{aligned} \bar{\phi}_f(E) &= S(E) \bar{\phi}_{fo}(E) \\ \bar{\phi}_m(E) &= S(E) \bar{\phi}_{mo}(E) \end{aligned} \quad (7)$$

If Eqs. (5) and (6) are added, we obtain:

$$\Sigma_{af} V_f \bar{\phi}_f(E) + \Sigma_{Tm} V_m \bar{\phi}_m(E) = V_m S(E), \quad (8)$$

which is just a neutron balance equation treating scattering in the moderator as removal and treating the source $S(E)$ as an external source.

The quantities $\bar{\phi}_{fo}(E)$ and $\bar{\phi}_{mo}(E)$ of Eq. (7) satisfy equations like Eq. (5) and Eq. (8), but with $S(E)$ replaced

by unity. These equations are

$$\Sigma_{Tf} V_f \bar{\rho}_{fo}(E) = \frac{\Sigma_{Tf}}{\Sigma_{Tm}} V_f P_f^* + V_f (1 - P_f^*) \Sigma_{sf} \bar{\rho}_{fo}(E) \quad (9)$$

$$\Sigma_{af} V_f \bar{\rho}_{fo}(E) + \Sigma_{Tm} V_m \bar{\rho}_{mo}(E) = V_m \quad (10)$$

Solving the equations for $\bar{\rho}_{fo}(E)$ and $\bar{\rho}_{mo}(E)$, we obtain

$$\bar{\rho}_{fo}(E) = \frac{\frac{\Sigma_{Tf}}{\Sigma_{Tm}} P_f^*}{\Sigma_{af} + \Sigma_{sf} P_f^*} = \frac{\frac{\Sigma_{Tf}}{\Sigma_{Tm}}}{\frac{\Sigma_{af}}{P_f^*} + \Sigma_{sf}} \quad (11)$$

$$\bar{\rho}_{mo}(E) = \frac{V_m \left(\frac{\Sigma_{af}}{P_f^*} + \Sigma_{sf} \right) - \Sigma_{af} V_f \frac{\Sigma_{Tf}}{\Sigma_{Tm}}}{\Sigma_{Tm} V_m \left(\frac{\Sigma_{af}}{P_f^*} + \Sigma_{sf} \right)} \quad (12)$$

If we define the disadvantage factor $d(E)$ by

$$d(E) = \frac{\bar{\rho}_m(E)}{\bar{\rho}_f(E)} = \frac{\bar{\rho}_{mo}(E)}{\bar{\rho}_{fo}(E)}, \quad (13)$$

then, from Eqs. (1) and (2),

$$d(E) = \frac{V_m \left(\frac{\Sigma_{af}}{P_f^*} + \Sigma_{sf} \right) - \Sigma_{af} V_f \frac{\Sigma_{Tf}}{\Sigma_{Tm}}}{\Sigma_{Tf} V_m} \quad (14)$$

It is interesting to relate this expression for $d(E)$ to the expression given by Sauer (Ref. 4). We make use of the approximation for P_f^* given by (Ref. 5)

$$P_f^* = \frac{P_o D}{1 - (1-D) (1 - \Sigma_{Tf} \bar{l}_f P_o)} = \frac{P_o D}{D + (1-D) \Sigma_{Tf} \bar{l}_f P_o} \quad (15)$$

where P_o is the escape probability from an isolated rod, D is the Dancoff factor ($D = 1 - C$, where C is the Dancoff correction), and $\bar{l}_f = 4V_f/S_f$ is the mean chord length for the fuel rod. With Sauer, we define the quantities $\tilde{H}_f$, $\tilde{H}_m$ by

$$P_o = \frac{1}{1 + \Sigma_{Tf} \bar{l}_f (1 + \tilde{H}_f)} \quad (16)$$

$$D = \frac{\Sigma_{Tm} \bar{l}_m}{1 + \Sigma_{Tm} \bar{l}_m (1 + \tilde{H}_m)}, \quad (17)$$

where $\bar{l}_m$ is the mean chord length for the moderator. From Eqs. (15), (16) and (17)

$$\frac{1}{p_f^*} = \frac{1}{p_o} + \left(\frac{1}{D} - 1 \right) \Sigma_{Tf} \bar{l}_f$$

or

$$\frac{1}{p_f^*} = 1 + \Sigma_{Tf} \bar{l}_f (1 + \tilde{H}_f) + \left(\frac{1}{\Sigma_{Tm} \bar{l}_m} + \tilde{H}_m \right) \Sigma_{Tf} \bar{l}_f \quad (18)$$

Using Eq. (18) in Eq. (14)

$$\begin{aligned} d(E) &= \frac{1}{\Sigma_{Tf}} \left(\frac{\Sigma_{af}}{p_f^*} + \Sigma_{sf} \right) - \frac{\Sigma_{af}}{\Sigma_{Tm}} \frac{v_f}{v_m} \\ &= \frac{1}{\Sigma_{Tf}} \left\{ \Sigma_{af} \left[1 + \Sigma_{Tf} \bar{l}_f (1 + \tilde{H}_f) + \left(\frac{1}{\Sigma_{Tm} \bar{l}_m} + \tilde{H}_m \right) \Sigma_{Tf} \bar{l}_f \right] + \Sigma_{sf} \right\} \\ &\quad - \frac{\Sigma_{af}}{\Sigma_{Tm}} \frac{\bar{l}_f}{\bar{l}_m} \end{aligned}$$

or

$$d(E) = 1 + \Sigma_{af} \bar{l}_f (1 + \tilde{H}_f + \tilde{H}_m) \quad (19)$$

Equation (19) gives the $d(E)$ obtained by Sauer, except that Sauer includes corrections $(\Delta H)_f$, $(\Delta H)_m$ for non-flat sources in the fuel and moderator.

If one substitutes $\bar{\rho}_{fo}(E) = \bar{\rho}_{mo}(E)/d(E)$ in Eq. (10), then one can obtain for $\bar{\rho}_{mo}(E)$ the equation

$$\frac{1}{\bar{\phi}_{mc}(E)} = \Sigma_{tm} + \Sigma_{af} \frac{V_f}{V_m} \frac{1}{d(E)} \quad (20)$$

From Eq. (7),

$$\frac{\bar{\phi}_{m_1}(E)}{\bar{\phi}_{m_0}(E)} = f(E) \quad (21)$$

so that, from Eqs. (20) and (21),

$$\left[\Sigma_{Tm_1} + \Sigma_{af} \frac{V_f}{V_m} \frac{1}{d(E)} \right] \bar{\phi}_{m_1}(E) = f(E). \quad (22)$$

Using the definition of $S(E)$, Eq. (4), one obtains

$$\left[\Sigma_{Tm_1} + \Sigma_{af} \frac{V_f}{V_m} \frac{1}{d(E)} \right] \bar{\phi}_{m_1}(E) = \int_0^\infty \Sigma_{sm}(E \leftarrow E') \bar{\phi}_{m_1}(E') dE' \quad (23)$$

Eq. (23) is of the form of an equation for the neutron spectrum in an homogeneous medium; it is seen that the equation may be interpreted as including the effect of the fuel by the use of a disadvantage-factor-weighted absorption cross section.

III. Determination of the Corrections to the HAMMER Resonance Absorption Model

If one makes use of the Cady approximation to the scattering kernel for hydrogen, then it turns out that the corrections to the HAMMER resonance absorption treatment which are required to account for thermalization effects are quite simple. At this point in the analysis, we assume that absorption in the water is negligible, and also neglect any interaction effects between smooth background absorption in the rod and the resonance absorption. We therefore, in the calculation of the resonance absorption, neglect the presence of the smooth background absorption cross section.

The Cady approximation to the hydrogen scattering kernel is to assume that the downscattering part of the kernel is the same as that due to scattering from a free proton at an effective temperature T^* . However, those neutrons which would upscatter in an effective temperature model are assumed to scatter without energy change. Moreover, for neutron energies on the order of 1 eV the scattering cross section for hydrogen is closely approximated by

$$\sigma_0(E) = \sigma \left(1 + \frac{kT^*}{\lambda E} \right) \quad (24)$$

where σ is the "high-energy limit" of the scattering cross section at energies above those for which thermal motion and chemical

binding effects are significant ($\sigma \approx 20.4$ barns). Furthermore, for scattering to energies E on the order of 1 eV from energies $E' > E$, the downscattering part of the effective temperature kernel may be approximated by

$$\sigma_0(E \leftarrow E') = \frac{\sigma}{E'} \quad (25)$$

The diagonal part of the Cady scattering kernel, obtained from the upscattering part of the effective temperature kernel, is

$$\sigma_{0,11}(E \leftarrow E') = \sigma \frac{kT^*}{E} \delta(E - E'). \quad (26)$$

With the help of Eqs. (24), (25), and (26), and keeping in mind the neglect of all absorption except the resonance absorption, we obtain from Eq. (23),

$$\left[\Sigma \left(1 + \frac{kT^*}{2E} \right) + \Sigma_{a,eff} \right] \bar{\phi}_m(E) = \Sigma \frac{kT^*}{E} \bar{\phi}_m(E) + \int_E^\infty \frac{\Sigma}{E'} \bar{\phi}_m(E') dE', \quad (27)$$

where Σ is the macroscopic scattering cross section of hydrogen in the high-energy limit (i.e., above energies where thermal motion and chemical binding effects are important),

and

$$\Sigma_{a,eff} = \Sigma_{af} \frac{V_f}{V_m} \frac{1}{d(E)} \quad (28)$$

Equation (27) is of the same form as that of the homogeneous spectrum problem for an absorber in hydrogen, with the protons considered to be free and at rest. It can therefore be solved in the same way. The solution is given in the paper by Cady et al. (reference 3), and may be written in the form

$$\bar{\Phi}_m(E) = \frac{f(E)}{5\Sigma_s + \gamma\Sigma_{a,eff}} \frac{1}{E} \quad (29)$$

where

$$f(E) = \exp \left\{ - \int_E^{\infty} \frac{dE'}{E'} \frac{\Sigma_{a,eff}}{5\Sigma_s + \gamma\Sigma_{a,eff}} \right\} \quad (30)$$

and

$$S(E)\Sigma_s(E) = \Sigma \left[1 + \frac{h\nu^*}{2E} \right]^2; \quad \Sigma_s(E) = \Sigma \left(1 + \frac{h\nu^*}{2E} \right) \quad (31)$$

$$\gamma(E) = 1 - \frac{h\nu^*}{2E} \quad (32)$$

It is easily verified that

$$\frac{dq}{dE} = \Sigma_{a,eff} \bar{\Phi}_m(E) = \Sigma_{af} \frac{V_f}{V_m} \frac{1}{f(E)} \bar{\Phi}_m(E) \quad (33)$$

$$= \frac{1}{V_m} \Sigma_{af} V_f \bar{\Phi}_f(E)$$

It follows from Eq. (33), and from the fact that $q(E) = 1$ for energies above the resonance (i.e., in the energy range $E_1 < E < \infty$ where $\Sigma_{af} = 0$), that $V_m q(E)$ gives the number of neutrons slowing down to energy E . Hence, the resonance escape probability is given by the value of q for energies below the resonance,

$$p = \exp \left(- \int_{res} \frac{\Sigma_{a,eff}}{\Sigma_s + \Sigma_{a,eff}} \frac{dE'}{E'} \right) \quad (34)$$

where the integral extends over the energy range of the resonance.

Denote the integral on the RHS of Eq. (34) by R , $p = \exp(-R)$. Then, using the definition, Eq. (28), of $\Sigma_{a,eff}$ we obtain

$$R = \int_{res} \frac{\Sigma_{af}(E')}{\int(E') \Sigma_s(E') d(E') \frac{V_m}{V_f} + \gamma(E') \Sigma_{af}(E')} \frac{dE'}{E'} \quad (35)$$

Approximate $\xi(E')\Sigma_s(E')$ and $\gamma(E')$ by their values at the resonance peak energy E_0 . Then, we may write R as

$$R = \frac{1}{f(E_0)\Sigma_s(E_0)} \frac{V_f}{V_m} \int_{res} \frac{\Sigma_{af}(E')}{d(E') + \frac{V_f}{V_m} \frac{\gamma(E_0)}{f(E_0)} \frac{\Sigma_{af}(E')}{\Sigma_s(E_0)}} \frac{dE'}{E'} \quad (36)$$

Let us examine the denominator of the integrand in Eq. (36). We have, using Eq. (19),

$$\begin{aligned} A &\equiv d(E') + \frac{V_f}{V_m} \frac{\gamma(E_0)}{f(E_0)} \frac{\Sigma_{af}(E')}{\Sigma_s(E_0)} \quad (37) \\ &= 1 + \Sigma_{af}(E') \bar{L}_f (1 + \bar{H}_f + \bar{H}_m) + \Sigma_{af}(E') \frac{\bar{L}_f}{\bar{L}_m} \frac{\gamma(E_0)}{f(E_0)\Sigma_s(E_0)\bar{L}_m} \\ &= 1 + \Sigma_{af}(E') \bar{L}_f \left[1 + \bar{H}_f + \bar{H}_m + \frac{\gamma(E_0)}{f(E_0)\Sigma_s(E_0)\bar{L}_m} \right] \end{aligned}$$

From Eq. (17),

$$\bar{H}_m = \frac{1}{D} - \frac{1}{\Sigma_s(E_0)} - 1. \quad (38)$$

Using Eq. (38) in Eq. (37), we have

$$A = 1 + \Sigma_{af}(E') \bar{L}_f \left[\bar{H}_f + \frac{1}{D} + \left(\frac{\gamma(E_0)}{f(E_0)} - 1 \right) \frac{1}{\Sigma_s(E_0)\bar{L}_m} \right] \quad (39)$$

If we had gone through the analysis neglecting thermal and chemical binding effects (i.e., had used a kernel corresponding to scattering from a free proton at rest) then we would have gotten the same results except that γ and ξ must everywhere be replaced by unity, and $\Sigma_s(E_0)$ must be replaced by Σ , the high-energy limit of the macroscopic scattering cross section of hydrogen. This means that the value of A would be replaced by

$$A_0 = 1 + \Sigma_{af}(E') \bar{L}_f \left[R_f + \frac{1}{D} \right] \quad (40)$$

and that the $1/(\xi(E_0) \Sigma_s(E_0))$ factor in front of the integral in Eq. (37) must be replaced by $1/\Sigma$. Comparing Eq. (39) with Eq. (40) we see that the effects of thermal motion and chemical binding on A can be taken into account by defining an effective Dancoff factor by

$$\frac{1}{D_{eff}} = \frac{1}{D} + \left(\frac{\gamma(E_0)}{\xi(E_0)} - 1 \right) \frac{1}{\xi(E_0) \bar{L}_n} \quad (40a)$$

In addition, the value of D must be computed with the water cross section given by $\Sigma_s(E_0)$. The correct slowing-down power $\xi(E_0) \Sigma_s(E_0)$ must be used in the R of Eq. (36).

According to this analysis the resonance escape probability in the absence of thermal motion and chemical

binding effect is given by $p_0 = \exp(-R_0)$, where

$$R_0 = \frac{1}{\Sigma} \frac{V_f}{V_m} \int \frac{\Sigma_{af}(E')}{A_0} \frac{dE'}{E'} \quad (41)$$

with A_0 given by Eq. (40). It is of interest to relate R_0 to the usual expression for the resonance integral in the wide resonance approximation (wide w.r.t. moderation in the fuel rod). The expression for the heterogeneous resonance integral in the wide resonance approximation as given by Dresner (ref. 6) reduces to

$$NI = \int P_{fa}^* \Sigma_{fa} \frac{dE}{E} \quad (42)$$

when all moderation in the fuel rod is neglected (i.e., all fuel scattering occurs without energy change). Here, N is the number density of the resonance isotope and P_{fa}^* is the non-absorption (not first-flight) escape probability. The resonance absorption (apart from effects taken into account by exponentiation) is given by

$$R_0' = NI V_f \bar{\phi} = NI V_f \frac{1}{\Sigma V_m} \quad (43)$$

per neutron slowing-down to the resonance. Here Σ is the hydrogen scattering cross section in the water.

The quantity R'_0 must be related to R_0 of Eq. (41). Making the spatially uniform collision density assumption Dresner shows that P_{fa}^* is related to the first-flight escape probability by

$$1 - P_{fa}^* = \frac{(1 - P_f^*)(1 - \frac{\Sigma_{sf}}{\Sigma_{tf}})}{1 - \frac{\Sigma_{sf}}{\Sigma_{tf}}(1 - P_f^*)} \quad (44)$$

from which one can obtain

$$\frac{1}{P_{fa}^*} = \frac{1}{\Sigma_{tf}} \left(\frac{\Sigma_{af}}{P_f^*} + \Sigma_{sf} \right) \quad (45)$$

Using Eq. (14) for $d(E)$, and identifying Σ_{Tm} with Σ , one obtains

$$\frac{1}{P_{fa}^*} = d(E) + \frac{\Sigma_{af}}{\Sigma} \frac{V_f}{V_m} \quad \text{so that}$$

$$R'_0 = N I V_f \frac{1}{\Sigma V_m} = \frac{1}{\Sigma} \frac{V_f}{V_m} \int \frac{\Sigma_{af}}{d(E) + \frac{\Sigma_{af}}{\Sigma} \frac{V_f}{V_m}} \frac{dE}{E} = R_0$$

We have therefore identified R_0 with the more usual expression for the resonance absorption R_0' . Note that the process of exponentiation of R_0 results in the removal of the error associated with the fact that the resonance is not completely narrow with respect to scattering by hydrogen.

References

1. A. J. Buslik, Nucl. Sci. Eng. 38, 72 (1969).
2. J. Chernick, "Proc. Intl. Conf. on Peaceful Uses of Atomic Energy", held in Geneva in 1955, Vol. 5, p. 215.
3. K. B. Cady, G. J. Kirouac, and J. J. McInerney, Nucl. Sci. Eng. 29, 299 (1967).
4. A. Sauer, J. Nuclear Energy, Parts A/B, 18, 425 (1964).
5. G. I. Bell and S. Glasstone, Nuclear Reactor Theory, Van Nostrand Reinhold Co., 1970 (p. 125).
6. L. Dresner, Resonance Absorption in Nuclear Reactors, p. 72 ff.
7. J. E. Suich and H. C. Honeck, "The HAMMER System", DP-1064 (1967).
8. S. Jabbawy, J. Karni, W. Rothenstein, and S. Velner, "Water Moderated Reactor Analysis with ENDF/B Data", IAEA/SM-170/8.