Calculation of fission product decay heat

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Calculation of Fission Product Decay Heat

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Abstract

A method is described for calculating decay schemes for nuclei far from the line of beta stability. Results of calculations of the decay heat using these calculated decay schemes are compared with experimental results.

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1. INTRODUCTION

There is a finite risk that water reactors loose their primary coolant. If this happens, the chain reaction and heat production are expected to cease promptly.

However, two sources of heat remain: The energy accumulated in the uranium fuel, and the radioactive fission products. A method to calculate the contribution from the latter source is described in the present report.

The heat from the radioactive decay of fission products - in short form called decay heat - depends on the density of the fission products in the reactor fuel and their decay schemes The calculation of decay heat is an easy task when the decay schemes are known. The problem is that decay schemes are not known for all fission products, especially not for those far from the line of beta stability. A method to calculate decay schemes for these nuclides is described together with the methods used to calculate the fission product density and the decay heat.

2. FISSION PRODUCT DENSITY CALCULATIONS

The density $N_i(t)$ of the fission product i at the time t is determined from the following set of coupled differential equations:

$$\frac{dN_i(t)}{dt} = -\hat{\lambda}_i N_i(t) + \sum_{j=1}^{nm} s_j(t) N_j(t) \quad i=1, 2, \cdots, nm. \qquad (2.1)$$

where

$\hat{\lambda}_i$ is the effective decay constant that is equal to the sum of the radioactive decay constant $\hat{\lambda}_i$ and the capture rate.

s_j^{nm}, is the source strength (fission rate times fission yield, activation rate, or radioactive decay).

The general solutions to the equations 2.1 are:

$$N_i(t+t_o) = N_i(t_o)e^{-\hat{\lambda}_i t} + e^{-\hat{\lambda}_i t} \int_{t_o}^{t_o+t} e^{\hat{\lambda}_i \tau} \sum_{j=1}^{nm} s_j(\tau) N_j(\tau) d\tau \qquad (2.2$$

$$i = 1,2, \quad ,nm$$

In reactor physics calculations t is of the order of 1-100 days. In the calculations of $N_i(t+t_o)$ made by means of the equations 2.2 t is divided into a number of time intervals Δt_k. The Δt_k's are chosen in the following way:

$$\Delta t_1 = t/2^n$$
$$\Delta t_2 = 2\Delta t_1$$
$$\vdots$$
$$\Delta t_n = 2\Delta t_{n-1}$$

and finally

$$t = \Delta t_n + \Delta t_{n-1} + \quad + \Delta t,$$

For the time interval Δt_k for which $s_j(\tau)\, N_j(\tau)$ is assumed constant, 2.2 is:

$$N_i(\Delta t_k+\Delta t_{k-1}+\cdots+\Delta t_1+t_o) = N_i(\Delta t_{k-1}+\cdots+\Delta t_1+t_o)e^{-\lambda_i \Delta t_k} + \frac{\sum_{j=1}^{nm} s_j N_j}{\lambda_i}(1-e^{-\lambda_i \Delta t_k}) \qquad i = 1,2,\ldots, nm \qquad (2.3)$$

$N_i(t+t_o)$ is calculated using 2.3 for the Δt_k's for k = 1, 2,...,n. n is calculated from the shortest half-life $T_{\frac{1}{2}}$ for the fission products treated in the density calculations and t in the following way:

$$n = \frac{\ln \frac{t}{T_{\frac{1}{2}}}}{\ln 2}. \qquad (2.4$$

3. DATA FOR THE DENSITY CALCULATIONS

A total of 563 different nuclides [8], including metastable states, are treated in the fission product calculations. Fission product yields and halflives are taken from [1] and capture cross sections are taken from the UK fission product library and transformed into 76-group cross sections. The capture cross sections

are not known for all fission products and are put equal to zero when unknown. The fission products with unknown cross sections are shortlived and the errors introduced by this assumption are therefore acceptable small. The 76-group cross sections are given in the library FPDATA.

4. DECAY HEAT CALCULATIONS

All the above-mentioned fission products decay by the emission of beta particles and the subsequent emission of gamma rays. The kinetic energy of the beta particles and the energy of the gamma rays is absorbed in the fuel and the cladding material, and the decay heat DH is calculated in the following way:

$$DH(t) = \sum_{i=1}^{nfp} \lambda_i N_i(t)\, q_i \qquad (4.1)$$

where

nfp is the number of fission products

q_i is the sum of the energy carried by the beta particles and the energy carried by the gamma rays.

The amount of energy carried by the gamma rays depends on the decay scheme of the nuclide i. The kinetic energy of the beta particles takes any value between zero and a maximum value, which depends on the energy of the excited levels in the daughter nuclide. The calculation of q_i, and also of DH, therefore demands knowledge of the decay scheme of the nuclide i and the spectrum of the kinetic energy of the beta particles.

5. DECAY SCHEMES

Decay schemes are known for 287 of the above mentioned 563 nuclides and they are taken from [2] and [3] and given in the library BGDATA. The nuclides with unknown decay schemes are short-lived, and to disregard them would introduce an error in the calculations of the decay heat for the first 100 seconds after shut-down of a reactor. Like other authors [6], we have tried to calculate a decay scheme for the nuclides with unknown decay schemes by calculating an average value of the ratio $\left(\frac{E_\gamma}{Q}\right)$

between the total decay energy Q and the average value of gamma energy $\bar{E}_\gamma$ from the 287 known decay schemes. This ratio is used to calculate the amount of energy carried by the beta particle and the amount of energy carried by the gamma quantum from the Q value. The result was

$$\overline{\left(\frac{\bar{E}_\gamma}{Q}\right)} = 0.35 \pm 0.25. \qquad (5.1)$$

However the above mentioned method was rejected because of the large uncertainty in the result. Decay schemes for the nuclides with unknown decay schemes were instead calculated in the way described below.

5.1 Decay schemes for nuclides far from the line of beta stability

All the nuclides with unknown decay schemes are far from the line of beta stability, and decay can proceed to a large number of excited levels. We therefore use a concept known from the theory of nuclear reactions, that of a strength function, to calculate the decay schemes.

The probability b(E) that a nuclide decays to the level at the energy Q-E by emission of a beta particle is:

$$b(E) = \frac{|M_{ij}|^2 \int_{m_o c^2}^{E} P(\grave{E})d\grave{E}}{\int_o^Q |M_{if}|^2 \int_{m_o c^2}^{E} P(\grave{E})d\grave{E}\, dE} \qquad (5.2)$$

P(E) is the probability that the beta particle is emitted with the energy E.

By means of 6.1, 5.2 is transformed into

$$b(E) = \frac{\frac{m_o^5 c^4 g^2}{2\pi^3 h^7} |M_{if}|^2 f(Q-E,Z)}{\frac{m_o^5 c^4 g^2}{2\pi h^7} \int_o^Q |M_{if}|^2 f(Q-\grave{E},Z)d\grave{E}} \qquad (5.3)$$

where

$$f(Q-E,Z) = \int_1^{\varepsilon^{max}} F(Z,\varepsilon)\ (\varepsilon^2-1)^{\frac{1}{2}}\ \varepsilon(\varepsilon^{max}-\varepsilon)d\varepsilon$$

m_o is the mass of the electron at rest,

c is the velocity of light,

h is the Planck's constant, and

g is a coupling constant.

M_{if}, is the integral over space of the product of the wave functions for the nucleus before decay, the initial state, and after decay, the final state. M_{if} depends on the maximum kinetic energy of the beta particle.

F(Z,ε) is a function that considers the coulomb interaction between the nucleus and the beta particle.

$$F(Z,\varepsilon) = k(Z)\,\frac{\varepsilon}{\varepsilon^2-1}$$

$$\varepsilon = \frac{m_o c^2 + E_\beta^{kin}}{m_o c^2} = \frac{E}{m_o c^2}$$

E_β^{kin} is the kinetic energy of the beta particle.

ε^{max} is the maximum value of ε, $\varepsilon^{max} = \frac{E}{m\,c^2}$ and

k(Z) is a function depending only on the atomic number z.

For a large number of excited levels, $|M_{if}|^2$ is written as $|M|^2\rho(E)$, where ρ(E) is the level density and where $|M|^2$ is an average value of the matrix elements.

By analogy with nuclear reaction theory, a beta strength function $S_\beta(E)$ is defined by

$$S_\beta(E) = \text{constant} \cdot |M|^2 \cdot \rho(E). \qquad (5.4)$$

It is known from [7] that $S_\beta(E)$ is zero below a cut-off energy E_c, and that it takes a constant value above this cut-off energy. E_c is equal to 0, $13/\sqrt{A}$ MeV, and $26/\sqrt{A}$ for even-even, odd mass and odd-odd nuclides respectively. A is the atomic weight.

By replacing $|M_{if}|^2$ by $|M|^2\rho(E)$ and using 5.4 and the above-mentioned characteristics of $S_\beta(E)$, equation 5.3 is transformed into

$$b(E) = \frac{f(Q-E,z)}{\int_{E_c}^{Q} f(Q-\grave{E},z)d\grave{E}} \quad . \tag{5.5}$$

An analytical expression is known for f(Q-E,z) and it is easy to calculate b(E) by means of 5.5

In the decay scheme calculations the number m of beta decay branches is quite arbitrarily chosen equal to the first integer larger than Q. The energy interval from 0 to Q is divided into subintervals with the boundaries $E_o = 0$, E_1, E_2.... $E_m = Q$, and the probability that a nuclide decays to levels at energy E with $E_j < E < E_{j-1}$ is

$$B_{j,j-1} = \frac{\int_{E_j}^{E_{j-1}} f(Q-\grave{E}, z)d\grave{E}}{\int_{E_c}^{Q} f(Q-\grave{E},z)\, d\grave{E}} \quad . \tag{5.6}$$

This means that we assume that the nuclide decays to levels energy $\frac{E_q+E_{j-1}}{2}$.

The decay scheme is established by assuming that the decay from an excited level to the ground state takes place by the emission of one gamma quantum.

6. THE KINETIC ENERGY OF THE BETA PARTICLES

The maximum value of the kinetic energy of the beta particles is known from the decay schemes and the kinetic energy of the beta particles is calculated using Fermi's theory of beta decay, which gives the following formula for the spectrum of the kinetic energy of the beta particle:

$$P(\varepsilon)\, d\varepsilon = \frac{m_o^5 c^4 g^2}{2\pi^3 h^7} |M_{if}|^2 P(Z,\varepsilon)\ (\varepsilon^2-1)^{\frac{1}{2}}\ (\varepsilon^{max}-\varepsilon)\varepsilon d\varepsilon \tag{6.1}$$

The amount of the kinetic energy of the beta particle, which is absorbed, is calculated as the average value of the

kinetic energy

$$\bar{\varepsilon} = \frac{\int_1^{\varepsilon^{max}} \varepsilon P(\varepsilon) d\varepsilon}{\int_1^{\varepsilon^{max}} P(\varepsilon) d\varepsilon} . \qquad (6.2)$$

Using the expression for $F(Z,\varepsilon)$ and the information of the energy dependence of $|M_{if}|^2$ given above, equation 6.2 is transformed into

$$\bar{\varepsilon} = \frac{\int_1^{\varepsilon^{max}} (\varepsilon-1)\varepsilon^2(\varepsilon^{max}-\varepsilon)^2 d\varepsilon}{\int_1^{\varepsilon^{max}} \varepsilon^2(\varepsilon^{max}-\varepsilon)^2 d\varepsilon} \qquad (6.3)$$

This formula 6.3 is used to calculated the average energy of beta particles absorbed in the reactor materials. The formula 5.6 is used to calculate the amount of energy carried by the gamma rays and the total amount of energy absorbed in the reactor materials, and the decay heat can now be calculated.

7. CALCULATIONS

Calculations of the decay heat from fission products formed by fission in ^{235}U due to a neutron burst of 10^{-4} seconds were performed, and the results of the calculations are shown in figure 1 together with experimental results taken from [9].

The calculated results for the decay heat show values below those of the experimental results from 0-100 seconds after the burst. The largest discrepancy of 15%, is found 1 second after the burst. The accuracy of the measurements is said in [9] to be 15%, and the calculated results and these experimental results are found to agree satisfactorily. A further evaluation of the described method of calculating the decay heat demands more accurate measurements.

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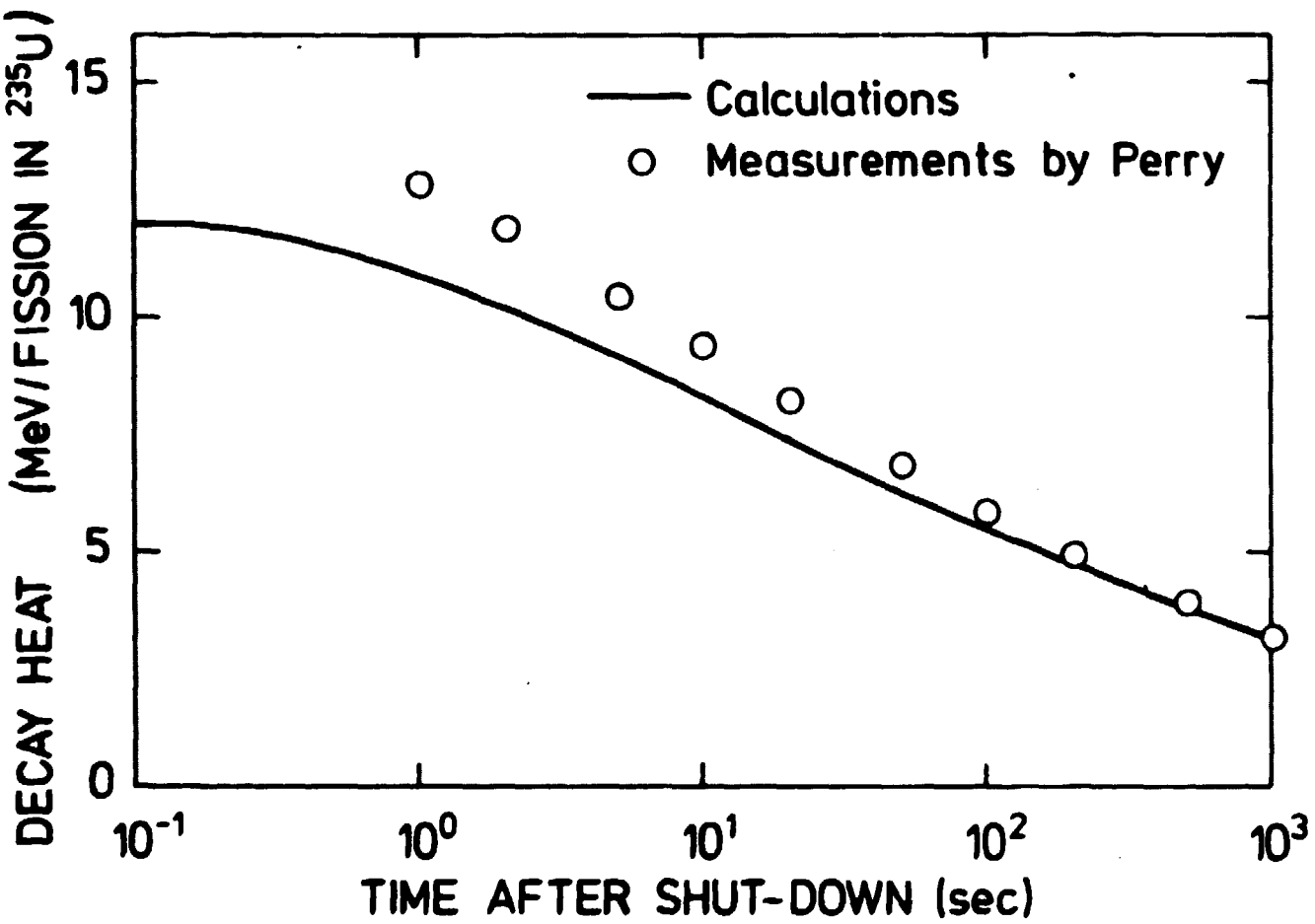

Fig. 1. Decay heat vs. the time after the burst (Reactor shut-down).