Annals of Nuclear Energy 57 (2013) 304–310

Contents lists available at SciVerse ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Numerical approach to calculate the decay heat of actinides for short cooling time

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ARTICLE INFO

Article history:
Received 23 September 2012
Received in revised form 12 February 2013
Accepted 14 February 2013
Available online 21 March 2013

Keywords:
Fission product
Decay heat
Numerical solution of linear differential equations

ABSTRACT

Calculations of the decay heat is of great important for the design of the shielding of discharged fuel, the design and transport of fuel-storage flasks and the management of the resulting radioactive waste. These are relevant to safety and have large economic and legislative consequences. In this paper, a new approach has been proposed to evaluate the decay heat power after a fission burst of a fissile nuclide for short cooling time. This method is based on the numerical solution of coupled linear differential equations that describe decays and buildups of the minor fission products (MFPs) nuclides. A computer program called HEATKAU is written entirely in the MATLAB programming environment. The MATLAB data can be stored in a standard, fast and easy-access, platform- independent binary format which is easy to visualize. Systematic comparisons with the measurements and the results evaluated by the summation method for ^{235}U and ^{239}Pu show the consistency and reliability of the current method.

1. Introduction

In an operating reactor, power is obtained following the nuclear transmutation of the fuel material, usually ^{235}U, and the subsequent conversion of mass to energy. The energy obtained in this fission process is divided among the kinetic energies of the fission products (including neutrons), energy of gamma radiation from "*prompt*" decay of highly-excited fission products, and finally the time-dependent beta- plus gamma-ray energy released following "delayed" decay of fission products (Nichols, 2002). This last-described source contributes about 7% of the total energy obtainable in the fission process (Gauld, 2006), and because of its time-dependent nature has been labeled "*Decay Heat*".

An accurate prediction of total decay heat and its time dependence is required in studies of loss of coolant accidents, and also in connection with the transportation and storage of spent fuel. At short cooling times, the main component is due to the decay of the fission products and also to ^{239}U and ^{239}Np decay, which are important for cooling times up to 15 days.

The importance of the different components of decay heat has been discussed in several papers (Tobias, 1980; Storrer, 1994). For shielding studies calculations of the gamma energy spectrum associated with the decay are also required. The gamma emission in beta decay of fission products is also an important component of the total gamma emission in normal reactor operation.

The evaluation of the decay heat has been recently performed by three methods. The basic method is the direct macroscopic measurement of the decay heat from a fissile nuclide after certain irradiation. The decay heat power after fast neutron induced fission for ^{232}Th, ^{233}U, ^{235}U, ^{238}U and ^{239}Pu has been measured at the fast neutron source reactor (YAYOI reactor) of university of Tokyo (England and Rider, 1994), whereas, that after thermal neutron induced fission for ^{235}U, ^{239}Pu and ^{241}Pu have been measured in Oak Ridge National Laboratory (ORNL) (Akiyama et al., 1982; Akiyama and An, 1982; Dickens and McConnell, 1980; Dickens et al., 1981). The second method is the summation (microscopic), in which the decay heat is calculated from the decay data and buildup of fission products (FPs) of a certain actinide (Yoshida et al., 1999; Ngoc Son and Jun-ichi, 2007). This method is based on summing of the activities of the fission products produced during the fission process and after the reactor shutdown weighted by the mean decay energies. The number of the atom nuclide i at cooling time t after burst fission ($N_i(t)$) can be calculated using an analytical formula. It has been reported that they used analytical methods without any simplification or approximation, in which all of linear and non-linear decay chains, and 12 decay modes, including ground state and meta-stable states, are automatically identified, and processed by using a decay data library and a fission yield data file to calculate the decay heat. The third one is the hybrid method that was reported by Oyamatsu et al. (2001). This method is based on the

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http://dx.doi.org/10.1016/j.anucene.2013.02.019

linearity of the decay heat to the fission yield. The coefficients of the linear combinations are obtained from fitting the fission yield of the given fissioning system with a linear combination of the fission yield of other fissioning systems with a residual term. This residual is calculated using the summation method of both the fission yields and the decay data. In other words, they approximate the fission yield vector of a fissioning system by a fission yield vectors of other fissioning systems and the coefficients of the linear combination are chosen such that to minimize the residual term. Then they used this residual term a as a correction term to validate the results obtained by their hybrid method to be in a reasonable consistence with the measured. The correction term is larger than 20% for several isotopes as listed in their paper. The agreement between the decay heat values obtained by this method and those measured are reasonable before 4000 s after shut down but not after that time. The discrepancy values for the total decay heat are up to 10% during the time region 300–3000 s.

In the present work, we proposed a new technique which uses three steps to evaluate the decay heat function. In the first step, we build the branching ratio, the decay constant and the independent fission yield matrices for the isotopes under consideration from the ENDF/B-VII.0 database. The second step concerning feeding those matrices into our inventory code which has been written in MATLAB 2012a, to calculate the number of nuclides after cooling time by solving the ordinary Bateman differential equations of initial value problem numerically using *Runge–Kutta* technique. This algorithm is used to reduce the truncation error in the calculation by taking large number of large steps which leads to a better accuracy for calculating the total decay heat over the time range 1–4000 s. It has been reported that a similar numerical algorithm is one of the advantages of the ALEPH Monte Carlo Simulation depletion (Stankovskiy and Van den Eynde, 2012). They have used the numerical solver for the first-order ordinary differential equations (ODEs) describing the isotope balances. It has been reported also, that the numerical algorithm speeds up the calculations of the ordinary differential equations unlike the matrix exponential method of which has been used in the ORIGEN-2.2 (CCC-371). This exponential method show weak dependence on the size of the ODE system and poor covariance properties of the method (Xie, 2011). In the last step of our approach, we used the ordinary summation method to calculate the decay heat.

2. Methodology

The calculation of the decay heat power is straight forward in the present approach once the input database is prepared. The input data required to calculate the fission products (FPs) decay heat are categorized into two. They are the fission-yield and decay data. The decay data consist of branching ratios (decay chains), half lives (decay constants) and average decay β- and γ- energies releases. These data are needed for about 1000 FP nuclides.

$$f(t) = \sum_i \overline{E}_i^{\beta,\gamma,\alpha}, \lambda_i, N_i(t) \tag{1}$$

where $f(t)$ is the power function (MeV/fission/s) following time t after a fission burst, $\overline{E}_i^{\beta,\gamma,\alpha}$ is the summation of the average β-, γ-, and α-energies per disintegration of nuclide I, which is given as $\overline{E}_i^{\beta,\gamma,\alpha} = (\overline{E}_{\beta,i} + \overline{E}_{\gamma,i} + \overline{E}_{\alpha,i})$. The average values of the β-, γ-energies were calculated from the decay schemes shown in Fig. 1, by the following relations; $\overline{E}_{\gamma,i} = \sum_i E_i I_i$ and $\overline{E}_{\beta,i} = \sum_i I_i \langle E_\beta \rangle_i$, where E_i is the gamma ray energy released per one beta decay, I_i is normalized beta-feeding to level I (Algora et al., 2010), and $\langle E_\beta \rangle_i$ is the mean energy of the β continuum populating level i. λ_i is the decay constant of the ith nuclide, and $N_i(t)$ is the number of nuclide i at cooling time

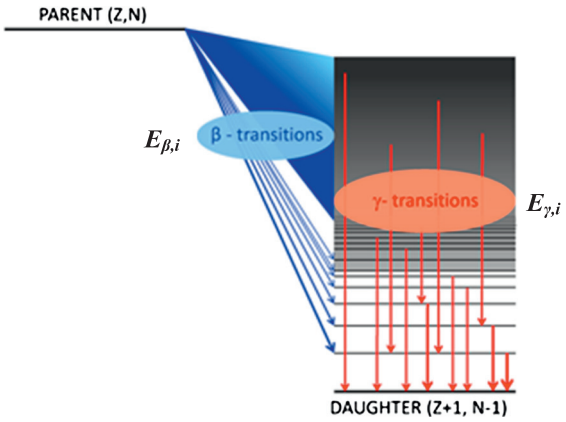

Fig. 1. A schematic diagram for a decay scheme to describe how to calculate the average energy of β- and γ-energies (Hardy et al., 1977).

t which is a numerical solution of coupled linear differential equations that describe decays and buildups of the MFP nuclides;

$$\frac{d}{dt}N_i(t) = -\lambda_i N_i(t) + \sum_j b_{j\to i}\lambda_j N_j(t) + Y_i \tag{2}$$

with

$$Y_i = \begin{pmatrix} N_1(0) \\ N_2(0) \\ N_3(0) \\ \vdots \\ N_M(0) \end{pmatrix} \tag{3}$$

Y_i is the matrix of initial independent fission yield of nuclide i and the index M is the number of fission products in the nuclide i. The $b_{j\to i}$ is the branching ratios matrix to nuclide i per decay of nuclide j;

$$b_{j\to i} = \begin{pmatrix} 0 & b_{2\to 1} & \cdots & b_{M\to 1} \\ b_{1\to 2} & 0 & \ldots & b_{M\to 2} \\ \vdots & \vdots & \ddots & \vdots \\ b_{1\to M} & b_{2\to M} & \cdots & 0 \end{pmatrix} \tag{4}$$

The decay constant λ_i can be represented in a form of diagonal matrix by;

$$\lambda_i = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_M \end{pmatrix} \tag{5}$$

The matrices in Eqs. (3)–(5) were extracted from the ENDF/B-VI.0 and fixed as inputs in the code with the option of updating whenever necessary for new decay data.

The *initial value problem* for an ordinary differential equation involves finding a function $N(t)$ that satisfies the condition

$$\frac{dN(t)}{dt} = f(t, N(t)) \tag{6}$$

together with the initial condition in Eq. (3). A numerical solution to this problem generates a sequence of values for the independent variable (Butcher, 2003; Brenan et al., 1996), t_0, t_1, …, and a corresponding sequence of values for the dependent variable, N_0, N_1, N_2, …, so that each N_m approximates the solution at t_m;

$$N_m \approx N(t_m), \quad t = 0, 1, \ldots \tag{7}$$