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TITLE: APPLICATION OF DETAILED FISSION-PRODUCT DECAY GAMMA SPECTRA
IN THE CALCULATION OF PHOTONEUTRON SPECTRA FROM $D(\gamma, n)$ REACTIONS
IN PWR FUEL

AUTHOR(S): W. B. Wilson, J. E. Stewart, T. R. England, and R. T. Perry

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Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

APPLICATION OF DETAILED FISSION-PRODUCT DECAY GAMMA SPECTRA
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REACTIONS IN PWR FUEL

W. B. WILSON, J. E. STEWART, AND T. R. ENGLAND
Los Alamos National Laboratory, Los Alamos, N.M., U.S.A.
R. T. PERRY
Texas A & M University, College Station, Texas, U.S.A.

Abstract The magnitude, average neutron energy, and spectrum of the photoneutron source in a PWR fuel is calculated for shutdown times to 100 y using CINDER radionuclide inventory calculations, ENDF/B-V γ line decay spectra, MCNP γ transport calculations, and PHONEX $D(\gamma,n)$ reaction physics calculations.

INTRODUCTION

Photoneutrons are produced in light water reactors by the interaction of energetic fission-product decay γ 's in (γ,n) reactions on deuterium naturally present in the water. Early calculations of the magnitude and spectra of photoneutron sources in thermal reactor fuels, summarized by Harris,¹ were limited primarily by the lack of evaluated decay γ spectra data for the radionuclides generated in the fuel. With the 1974 release of the fission-product data file of ENDF/B-IV,² much of this data became available. This file contained evaluated cross sections, direct and cumulative fission yields, and a range of decay data including half-lives, branchings, Q values, and decay spectra for α 's, β 's, γ 's and discrete electrons. The evaluated fission-product decay γ spectra for 32 of the 58 fission products with γ 's exceeding the $D(\gamma,n)$ 2.23-MeV threshold, were used by Stametelatos and England in PHONEX³ code calculations with evaluated $D(\gamma,n)$ cross-section data to calculate temporal photoneutron source spectra.⁴ These calculations used the γ spectra, processed into 66 energy bins, with temporal radionuclide inventories calculated with CINDER⁵ for each of 10 yield sets of ENDF/B-IV to form aggregate γ spectra for a variety of irradiation and shutdown scenarios. These aggregate γ source spectra were used to calculate photoneutron spectra with PHONEX, which assumed that the γ flux spectrum in the deuterium-containing water was proportional to the γ source spectrum in the fuel. (Reference 4 also contains similar calculated results for $^9\text{Be}(\gamma,n)$ photoneutron production.)

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CALCULATIONS WITH ENDF/B-V DATA

We have now improved upon this procedure using the more extensive ENDF/B-V² fission-product data released in 1980. ENDF/B-V spectra have been used with radionuclide inventories calculated with CINDER and an ENDF/B-V based library for an actual PWR fuel, MCNP⁶ Monte Carlo γ transport calculations of source γ 's in the Zirc-4 clad UO₂ fuel rod and water lattice, and D(γ ,n) reaction physics calculations with an improved PHONX84 version of the PHONEX code.

ENDF/B-V Decay γ Spectra Data

The fission-product data files include γ decay spectra data for 247 nuclides, including 86 having γ 's with energies in excess of 2.23 MeV; the maximum γ energy of the file is 6.99 MeV. A nominal 0.25-MeV grid of 20 γ energies from 2.23 MeV to 7 MeV was defined for use in photon-neutron calculations. The decay γ line energies and intensities for all 86 nuclides, including only the epi-threshold γ 's, were isolated in a unit decay γ spectra file.

CINDER Radionuclide Inventory Calculations

CINDER inventory calculations were made for 2.56% initial enrichment fuel discharged from H. B. Robinson-2 at 31.5 GWd/tU. Previous benchmark calculations of this fuel, using exposure-dependent resonance self-shielded actinide cross sections and temporal 4-group fluxes from companion EPRI-CELL calculations modeling a cell of the 15 x 15 assemblies have been described in Ref. 7. The library of ENDF/B-V data developed for the CINDER calculations has been described in Ref. 7. From the CINDER results a file of fuel inventories was formed for the 86 fission products, giving atom densities (atoms/cm³ fuel) at shutdown and 47 cooling times ranging from 0.1 s to 100 y.

MCNP γ Transport Calculations

The geometry of the PWR clad fuel rod and water lattice was modeled for transport calculations as a cubic cell centered on one axis about a clad fuel rod with pellet o.d. of 0.934 cm and clad o.d. of 1.074 cm. Each edge of the cell measured 1.43 cm, equal to the rod pitch, and all outside boundaries were reflecting. Element atom densities for the fuel were taken from the CINDER-calculated discharge inventory, using ⁴¹NB and ⁵⁹PR to represent the light- and heavy-mass fission products, respectively. Clad element atom densities were taken from the EPRI-CELL engineering data for Zirc-4. Water atom densities were taken from an assumed 1 g/cm³ density, appropriate for discharged fuel calculations but about 40% high for operating conditions. Separate MCNP calculations were made for each γ energy on the grid, each with 100 000 source γ 's started in the fuel from an isotropic and homogeneous source description. The γ track length of each transported γ was binned by γ energy group and material, with the largest statistical uncertainty in any group track length in water for any source energy found to be 6.35%. The γ

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energy-binned track lengths in water for each γ source energy were divided by the source strength (100 000 γ 's) to produce a file of unit source γ energy-binned track lengths in water.

PHONX84 Calculations

The original PHONEX³ code uses input γ energy-binned source spectra (assumed proportional to flux, fluence, or track lengths) and input photoelectric and photomagnetic cross sections to calculate photoneutron spectra, using isotropic photomagnetic and \sin^2 photoelectric neutron angular distributions in the center-of-mass system. The code includes energy and angle transformations to and from each system; γ track lengths are assumed uniformly distributed in energy within each γ group. However, the code has cumbersome IO and provides no method of inputting target atom densities. A modified version PHONX84 was used with deuterium photoneutron cross section data of the earlier calculations⁴ and the light water deuterium atom density, taking deuterium at 150 ppm $_1\text{H}$, to calculate unit γ water track length photoneutron spectra in 100-keV bins.

RESULTS

The files from each activity described above were retained for the greatest flexibility of application. For these aggregate photoneutron calculations, the unit decay γ line spectra file of reduced ENDF/B-V data was first used (by interpolation) with the file of unit source γ energy-binned track lengths in water reduced from MCNP results to produce a file of unit decay water track lengths for each of the 86 fission products. This file was, in turn, combined with the file of unit γ water track length photoneutron spectra produced from PHONX84 calculations, producing a file of unit decay photoneutron spectra for each of the 86 fission products. This file was then combined with nuclide decay constants and the fission product inventory file to calculate the magnitude, shown in Figure 1, and spectra, shown in Figure 2, of the photoneutron source in the fuel at each cooling time. The photoneutron source was found to be negligible (<1 n/s/cm³ fuel) at cooling times beyond a few thousand hours.

This photoneutron spectra calculation capability complements the (α ,n), spontaneous fission, and β ,n delayed neutron spectra calculation capabilities of the SOURCES code.⁹

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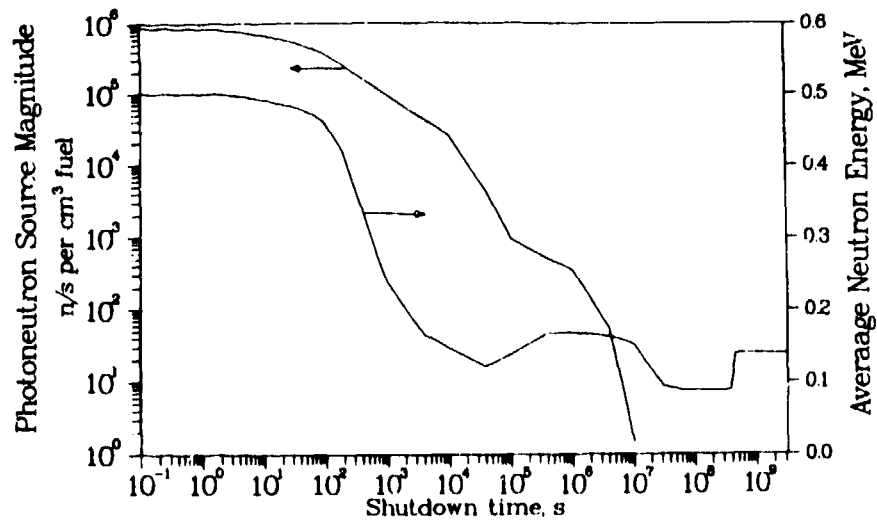


FIGURE 1 Photoneutron source magnitude and average neutron energy of discharged 31.5 Gwd/tU 2.56% H. B. Robinson-2 PWR fuel.

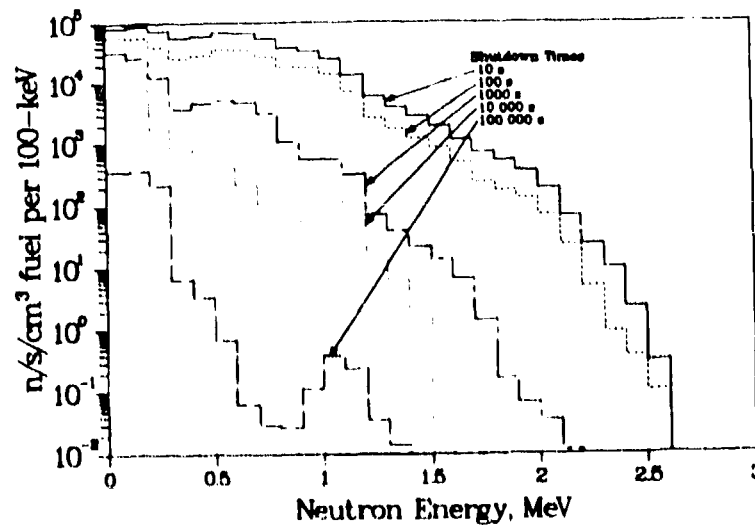


FIGURE 2 Photoneutron spectra of discharged 31.5 Gwd/tU 2.56% H. B. Robinson-2 PWR fuel.