ORIGEN-S Gamma Decay Spectra Characterization and Benchmarking

J.J. Klingensmith, I.C. Gauld

Pennsylvania State University, 138 Reber Building, University Park, PA 16802, jxk390@psu.edu
Oak Ridge National Laboratory, P.O. Box 2008, MS 6370, Oak Ridge, TN 37831, gauldi@ornl.gov

INTRODUCTION

This works describes validation studies recently performed for the updated version the revised ORIGEN-S master photon library released with SCALE 5.0. Validation was performed by comparing predicted gamma spectra from ORIGEN-S against experiment.

The photon library released with previous versions of the SCALE package contained data for 418, mostly longer-lived, nuclides. The data library was developed in the late 1970's from the Evaluated Nuclear Data Structure File (ENSDF) and left relatively unchanged for nearly 25 years. The library has been shown to be adequate to calculate gamma emission and gamma heating at times longer than several hours, which was sufficient for ORIGEN-S's major function in SCALE; the analysis of shipping casks for spent nuclear fuel. Improvements in nuclear data evaluations motivated an update of the existing photon library with many additional nuclides and more comprehensive photon data.

The revised master photon library (MAPH) released with SCALE 5 dramatically increased the number of nuclides, from 418 to 2101, as well as the number of discrete photon lines, from 12,000 to 115,000. The majority of the new isotopes are short-lived and the level of detail in the photon libraries has been increased throughout the library.

In order to quantify the accuracy of the new photon database, a benchmarking exercise was performed using experiments were performed at Oak Ridge National Laboratory circa 1979. [1]. Measured gamma-ray spectra were available for small, nearly pure, samples of ^{235}U, ^{239}Pu, and ^{241}Pu following irradiation in a thermal flux. The spectra were then measured for times between 2.7 and 14000 seconds after fission has ceased.

These experiments were simulated using ORIGEN-S using both the new and old photon libraries. For comparison, the libraries are referenced here by the package that they were released with, i.e. the old MAPH is labeled SCALE 4.4 and the new MAPH is labeled SCALE 5.

METHODS AND CODES

ORIGEN-S is a decay and depletion code that is included in the SCALE code package. ORIGEN-S is used primarily for analysis of nuclide compositions, decay heat, and radiation sources from spent nuclear fuel [2]. The accuracy of the results is largely dependant on the quality of the nuclear data used for the calculations. The following results are intended to test the quality of the recently updated photon release data.

The photon libraries used by ORIGEN-S contain discrete photon line energies and yields per disintegration. Thus, the code will calculate spectra in any user-desired group structure. The updated photon library was compiled from the evaluations of ENDF/B-VI, ENSDF, and JEF-2.2.

PRELIMINARY RESULTS

The initial results compared the output of ORIGEN-S using the SCALE 4.4 MAPH and the SCALE 5 MAPH with the experimental results. The predicted spectra were normalized to gamma rays per fission to match the measured data from experiment. The ORIGEN-S data were calculated in energy bins matching those of the experimental data points to better compare the results. However, in order to obtain reasonable comparisons the spectra predicted by ORIGEN-S had to be broadened to match the energy-resolution of the gamma detectors used in the experiment. The detector resolution was well-characterized in the experiment, allowing the energy response to be accurately simulated.

This was simulated by calculating the spectra using a very fine energy increment and applying a Gaussian distribution to the results.

Initial results with the SCALE 5 library indicated that the total gamma energy associated with the spectra was larger than the energy predicted on the basis of Q values. Further investigation found that many gamma lines were double accounted as a result of being included twice in decays leading to a metastable state daughter product. The library was later processed to eliminate the duplicate lines.

RESULTS

Figures 1 through 3 show the measured and predicted gamma spectra as a function of time after

fission. At the shortest count times, the SCALE 4.4 library is obviously missing the majority of the gamma ray emission, while the SCALE 5 libraries account for 99.9% of the energy release. Note that ORIGEN-S normally renormalizes the gamma spectra such that the gamma energy of the spectra is equal to that predicted on the basis of Q values. In this study the spectrum normalization of turned off to more easily evaluate the quality of the photon data.

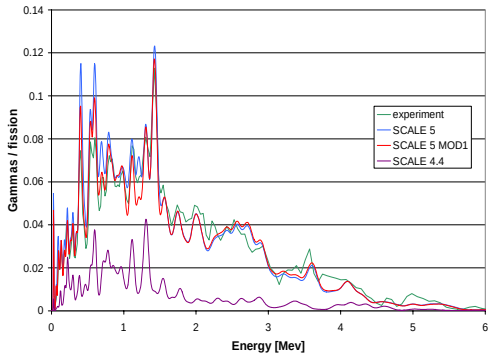

Fig. 1. Calculated and experimental gamma spectra 2.7 seconds after U-235 fission.

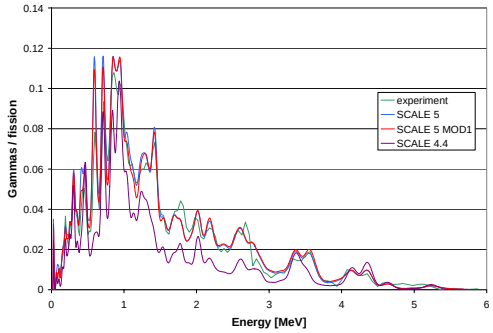

Fig. 2. Calculated and experimental gamma spectra 35 seconds after U-235 fission.

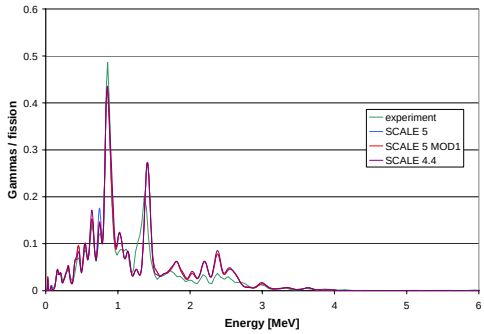

Fig. 3. Calculated and experimental gamma spectra 9950 seconds after U-235 fission

The SCALE 4.4 results are seen to improve with increasing decay time as the longer-lived fission products become increasingly dominant. The spectra predicted using the revised library in SCALE 5 are observed to be in good agreement with experiment for all times, including the shortest cooling time of 2.7 seconds after fission.

CONCLUSIONS

The immediate conclusion is that the revised photon library greatly improves the predicted spectra at short times. Even at the shortest count times, the gamma energy release calculated in ORIGEN-S and the experimental value agree to within 1%. The shapes of the calculated spectra are also in excellent agreement with the experimental spectra. The results for all three fissile isotopes studied were found to be consistent with those presented here for ^{235}U, leading to increased confidence that the ORIGEN-S spectral can be applied confidently at extremely short cooling times after fission.

The revised photon library also includes many more activation products that were previously omitted.

REFERENCES

1. J. K. Dickens, T. A. Love, J. W. Connell, K. J. Northcutt, R. W. Peelle, and H. Weaver, “Delayed Beta- and Gamma-Ray Production due to Thermal-Neutron Fission of ^{235}U: Spectral Distributions for Times After Fission Between 2 and 14,000 Seconds (tabular and graphical data),” Oak Ridge National Laboratory report ORNL/NUREG-39 (NUCREG/CR-0162), 1978.
2. I. C. Gauld, O. W. Herman, and R. M. Westfall, “ORIGEN-S: SCALE System Module to Calculate Fuel Depletion, Actinide Transmutation, Fission Product Buildup and Decay, and Associated Radiation Source Terms,” Vol. II, Sect. F7, ORNL/NUREG/CSD-2/V2/R7 (draft).