Validation of SCALE SAS2H Isotopic Predictions for high burnup PWR spent fuels

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1. Introduction

A precise prediction of the time-dependent radionuclide inventory in a spent fuel is an essential step to evaluate many spent fuel related issues, including a neutron multiplication for criticality safety problems, neutron and gamma-ray sources for a radiation shielding and a dose rate analysis, decay heat sources for a thermal analysis, and radiological and chemical toxicity terms for environmental impact considerations. One of the important functions of the SCALE (Standardized Computer Analyses for Licensing Evaluation) code system is its capability to predict the an isotopic composition of a depleted fuel discharged from a PWR fuel.[1] To validate the codes and data used in depletion approaches, experimental measurements are compared with numerical predictions for relevant spent fuel samples. Such comparisons have been carried out in earlier works at the Oak Ridge National Laboratory. However, the majority of the previous works were performed in a range below 45 GWd/MTU using SCALE 4.x system.

PIEF (Post Irradiation Examination Facility) in KAERI (Korea Atomic Energy Research Institute) recently performed radiochemical analyses and has obtained the radiochemical measurement assay from seven spent fuel samples which were obtained from commercial Korean PWR plants, Ulchin unit 2 and Yonggwang unit 1. The burnup of these spent fuel samples is between 38.03 to 59.78 GWd/MTU. The isotopic composition of these spent fuel samples was calculated by the SAS2H control module contained in the SCALE 5.1 system. Then, comparisons between the calculated and measured isotopic compositions for high burnup PWR spent fuel samples were carried out.

2. Methods and Results

2.1 Fuel and Assembly Specifications

Spent fuel samples used in this study were obtained from commercial Korean PWR plants, Ulchin unit 2 and Yonggwang unit 1. Uljchn unit 2 and Yonggwang unit 1 are pressurized water reactors with a power rating of 900 MWe and 1000 MWe, respectively and operate with assemblies having a 17×17 Westinghouse type fuel lattice design.

Spent fuel samples were obtained from three assemblies, K23, O59 and P09. K23 and O59 were irradiated for 3 cycles in Ulchin unit 2 and Yonggwang unit 1, respectively. P09 was irradiated for 2 cycles in Yuongkwang unit-1. Radiochemical analyses were performed for seven spent fuel samples obtained from one rod in each assembly. Seven samples were taken from various axial locations of three fuel rods. Spent fuel samples covered a high burnup range, from 38.03 GWd/MTU to 59.79 GWd/MTU.

2.2 Experimental Measurements and Methods

Radiochemical analysis of the spent fuel samples was performed to determine the isotopic compositions of U, Pu, and Nd. And the burnup of the spent fuel samples was determined experimentally by the Nd-148 method. The use of Nd-148 as a burnup monitor for a nuclear fuel is generally accepted as a standard method since the issue of the ASTM E321-69.[2] For a burnup measurement, Nd is usually separated from the spent fuel samples and its amount is determined by the mass spectrometric isotopic dilution technique. Isotopic compositions of the U, Pu, and Nd in the spent fuel samples with and without a spike addition were determined by the sequential anion and cation exchange separation procedures. Isotopic compositions that had been isolated and concentrated were measured by using TIMS (Thermo-Ionization Mass Spectroscopy).

After the mass spectrometric measurement of each portion isolated from the spiked and unspiked sample solutions, the isotopic concentrations of U, Pu, and Nd in the sample solutions were determined by IDMS (Isotopic Dilution Mass Spectroscopy).

2.3 Depletion Analysis

The depletion calculations were carried out using the SAS2H control module in Version 5.1 of the SCALE code system. SAS2H is a multi-code sequence that determines the isotopic composition of a spent fuel using the ORIGEN-S code for the depletion and decay calculations and a one-dimensional neutronics model of a LWR fuel assembly to prepare the burnup-dependent cross sections for ORIGEN-S.[3]

The nature of the neutron cross-section data used in the fuel depletion analyses by the SCALE system is a significant aspect for a validation effort. In these analyses, a 44-group cross section library was applied. The 44-group library applied in these analyses was derived from ENDF/B-V data. And because of the large guide tubes in the Westinghouse 17×17 fuel assembly design, a "path-B" model for the SAS2H calculations was applied to describe a larger unit cell as a guide tube surrounded by the fuel.

It was assumed that the heat produced in the coolant versus the fuel height was a sine function.[4] Integrating this function yields the following formula for the coolant temperature versus the height:

$$T(h) = T_{IN} + \frac{T_{OUT} - T_{IN}}{2}\left(1 - \cos\frac{\pi h}{H}\right)$$

where T(h) : temperature at height h,
T_{IN} : inlet temperature,
T_{OUT} : outlet temperature,
H : active fuel length.

The coolant density was determined by using these temperatures to interpolate them into a standard temperature-pressure-density table at a pressure of 2250 psia.[5] The average fuel temperature was estimated approximately from the analytic solutions as a function of the linear power for the reactor rod data. And the depletion calculation performed in this analysis used an average boron concentration of 800 ppm.

The unit of the calculated data for U, Pu, and Nd isotopes from SAS2H was converted to a unit of g/g-element to allow for the predictions to be compared more directly with an analysis performed at a unit of mass/MTU.

2.4 Results

The percentage differences between the measured and calculated concentrations for each isotope of the corresponding samples are shown in Fig. 1.

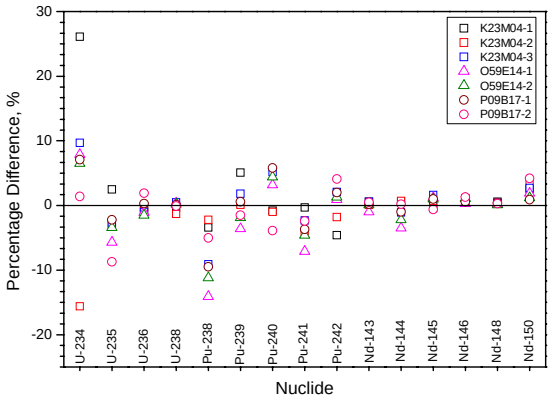

Fig. 1. Percentage difference[(calculated-measured-1)×100] of U, Pu, and Nd isotopes for seven spent fuel samples

The average percentage differences for the U isotopes are 6.2 % for U-234, −3.3 % for U-235, −0.4 % for U-236, and –0.1 % for U-238. With the exception of U-234, U isotopes results are generally consistent with earlier studies. In general, the prediction of the nuclide inventories for the uranium isotopes is within about 1%, with the exception of U-234, which is generally predicted in the range of 2 to 6%. This relatively broad variation may result from the correlation used to estimate the initial loading of U-234 isotope, since these data are not generally provided directly in available references.[6]

The average percentage differences for the Pu isotopes are –7.8 % for Pu-238, 0.1 % for Pu-239, 1.8 % for Pu-240, –3.5 % for Pu-241, and 0.6 % for Pu-242. Predictions for the Pu isotopic concentrations vary by isotope. Pu-238 reveals the largest variation between measurements. This may be partly due to the small amount of each nuclide present in a spent fuel relative to the other plutonium nuclides. According to earlier works, Pu-239, Pu-240, and Pu-241 are predicted in the order of within between 1 to 2% based on calculations using a 44-group library.[6] In this study, Pu isotopes results are in good agreement with these earlier studies except for Pu-238.

The average percentage differences for the Nd isotopes are 0.2 % for Nd-143, –0.9 % for Nd-144, 0.6 % for Nd-145, 0.9 % for Nd-146, 0.3 % for Nd-148, and 2.4 % for Nd-150. Nd isotopes reveal a small variation between the measurements. And these results are also consistent with previous works.

3. Conclusions

Comparisons of the calculated and measured isotopic compositions for high burnup Korean PWR spent fuel samples were performed and the difference was shown to be within a few percent. These results are not only in good agreement with earlier studies, but also reasonably good estimates. But a validation for additional nuclides, such as fission products and the major actinide nuclides, should also be performed.

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