Evaluation and Validation of New Cross Section and Covariance Data for AFC Applications

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1. Introduction

International collaboration between KAERI and ORNL has been carried out under the International Nuclear Energy Research Initiative (I-NERI) project since 2008. The main goal of the collaboration is to provide improved neutron cross section data with covariance data for isotopes important for the advanced fuel cycle (AFC) and nuclear safeguards applications. After comprehensive analyses for the AFC and safeguards applications, ²³⁷Np, ²⁴⁰Pu, and Cm-isotopes were selected as priority nuclides, which have been needed for improvements due to oldness of evaluations available in ENDF/B-VII.0, JEFF-3.1.1, and JENDL-3.3.

Up to now preliminary evaluations of cross section with covariance data have been produced for ²³⁷Np, ²⁴⁰Pu, and Cm-isotopes under the collaboration. In particular, the evaluation for ²⁴⁰Pu has been completed just at the moment. In this paper, the cross section and covariance data evaluations for the actinide nuclides are briefly described. In addition, the criticality benchmark calculation results of the new ²⁴⁰Pu cross section and covariance data are compared with those based on recent evaluations such as ENDF/B-VII.0, JEFF-3.1.1, and JENDL-4.0.

2. Cross Section and Covariance Data Evaluation

The new ²⁴⁰Pu was obtained by replacing the ENDF/B-VII.0 resonance parameters with the new resonance parameters and by adding the Resonance Parameter Covariance Matrices (RPCMs). The new resonance parameters and RPCMs generated by ORNL and the high-energy cross section and covariance data evaluated by KAERI for the ²⁴⁰Pu were combined to a complete ENDF-format file. The ²⁴⁰Pu neutron capture cross section and correlation matrix is provided in Figure 1. The objective of the ²⁴⁴Cm evaluation effort is to provide resonance parameter covariance data while preserving the existing resonance parameter data in File 2 of the cross section evaluation. Moreover, the resonance parameter covariance evaluation will be used to complement the high-energy cross section and covariance analysis work being performed by KAERI for the Cm isotopes. In the ORNL work, the RPCMs based on the resonance parameters of the JENDL-4.0 evaluation were generated for ²⁴⁴Cm using the SAMMY R-Matrix software in the energy range from 10^{-5} eV to 1 keV. The retroactive approach of the SAMMY software was used to generate the RPCM for ²⁴⁴Cm.

KAERI has completely re-evaluated the cross section data and covariance matrix above resonance energy for ²⁴⁴Cm with EMPIRE/KALMAN software.



Fig. 1. New $^{\rm 240}{\rm Pu}$ capture cross section and correlation matrices.

3. Criticality Benchmark for ²⁴⁰Pu Cross Section and Covariance Data

3.1 Benchmark Problem

The criticality safety benchmark problems containing ²⁴⁰Pu were selected from the ICSBEP and/or CSEWG specifications [1]. These problems are composed of 22 fast assemblies and 6 thermal assemblies for validating the new cross section data in resonance and high energy region. The fast benchmark problems are classified by various reflector materials such as beryllium and beryllium oxide, steel and nickel, normal uranium, and so on. The thermal benchmark problems are a series of PNL experiments with different concentrations of plutonium nitrate solution.

For most benchmark problems, the effects of the 240 Pu covariance data are hardly seen due to the small contribution to the k_{eff} estimation. In this study, two criticality safety benchmark problems such as Pu239-JEZEBEL (PU-MET-FAST-001) and Pu240-JEZEBEL (PU-MET-FAST-002), which contain a relatively large amount of 240 Pu, were selected to validate the covariance data of 240 Pu. Especially for Pu240-JEZEBEL with 20.1% 240 Pu, more apparent impacts due to relatively high 240 Pu content are expected on the uncertainty estimation than Pu239-JEZEBEL with 4.5% 240 Pu.

3.2 Validation of Cross Section Data

All the benchmark calculations have been performed with the MCNP code and compared with the

measurements. The impacts from the recent ²⁴⁰Pu evaluations of KAERI/ORNL, JEFF-3.1.1, and JENDL-4.0 have been estimated by replacing only the ²⁴⁰Pu data in the ENDF/B-VII.0-based reference calculations. Figures 2 and 3 show the comparisons of the k_{eff} results produced from different ²⁴⁰Pu evaluations for fast and thermal critical assemblies, respectively. Most of the calculation results generally agree well with the measured k_{eff}'s within around 1000 pcm except for a few benchmark problems, while these recent ²⁴⁰Pu evaluations show a similar trend for each benchmark problem. In addition, the fast benchmark results, as depicted in Figure 2, show a better sign for the KAERI/ORNL data than the ENDF/B-VII.0 data. On the whole, the 240 Pu data of JENDL-4.0 tends to produce better results than others in our selected benchmark problem set.



Fig. 2. Comparisons of k_{eff} results for fast critical assemblies.



Fig. 3. Comparisons of $k_{\rm eff}$ results for thermal critical assemblies.

3.3 Validation of Covariance Data

A discrete ordinates-based DANTSYS/SUSD3D [2] code system has been taken into consideration for the nuclear data sensitivity and uncertainty analysis of k_{eff} . The neutron cross section and its covariance data of ²⁴⁰Pu based on the JENDL-3.3 are considered as a reference dataset in the sensitivity and uncertainty analysis of the k_{eff} against the other evaluations. The uncertainties originating from the covariance data of JENDL-3.3 were estimated, and then the impact of the use of ²⁴⁰Pu covariance data from the other evaluations was analyzed by replacing the covariance data of JENDL-3.3 with those of Low-Fidelity, JENDL-4.0, or KAERI/ORNL data.

The total uncertainties from the reference dataset were calculated to be 0.467% and 0.511% for the

Pu239-JEZEBEL and Pu240-JEZEBEL, respectively. For the Pu239-JEZEBEL, the impact of the use of the different ²⁴⁰Pu covariance data was insignificant, which was mainly come from the small contribution of the 240 Pu data to the k_{eff} estimation. The Pu240-JEZEBEL with relatively high ²⁴⁰Pu content shows about 0.1% of increase for the Low-Fidelity covariance data in the total uncertainties of keff, whereas it shows about 0.1% of decrease for the JENDL-4.0 and KAERI/ORNL covariance data. The former increase is attributed to the large uncertainties of the fission covariance data of ²⁴⁰Pu from the Low-Fidelity data and the latter decrease is attributed to the small uncertainties of the $\overline{\nu}_{\tau}$ (MT=452, average total number of neutrons released per fission event) covariance data of ²⁴⁰Pu from the JENDL-4.0 and KAERI/ORNL data. Figure 4 shows the k_{eff} uncertainty variations by $^{\rm 240}\mbox{Pu}$ nuclear reactions for the Pu240-JEZEBEL critical system.



Fig. 4. Total k_{eff} uncertainty variations by ²⁴⁰Pu nuclear reactions for Pu240-JEZEBEL critical system.

4. Summary

The neutron cross section data with covariance data have been generated for ²³⁷Np, ²⁴⁰Pu, and Cm-isotopes under the collaboration between KAERI and ORNL. The complete evaluations for ²⁴⁰Pu have been validated via appropriate criticality safety benchmark calculations. A slight improvement of reaction cross sections in fast energy region has been observed for the new KAERI/ORNL evaluation. In terms of covariance data, the new KAERI/ORNL evaluation was comparable to the latest JENDL-4.0 data for the most part.

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REFERENCES

[1] J. B. Briggs, "International Handbook of Evaluated Criticality Safety Benchmark Experiments," *NEA/NSC/DOC(95)03*, Nuclear Energy Agency, OECD (2007).

[2] I Kodeli, "SUSD3D: A Multi-Dimensional, Sensitivity and Uncertainty Analysis Code System," *NEA-1628/02*, Nuclear Energy Agency, OECD (2006).