A stress test on $^{235}\text{U}(n, f)$ in adjustment with HCl and HMI benchmarks

Haicheng Wu$^{1,\ast}$, Yingcan Qin$^1$, and Massimo Salvatores$^2$

1 China Nuclear Data Center, China Institute of Atomic Energy, PO Box 275-41, Beijing 102413, China
2 Idaho National Laboratory, Idaho Falls, ID, USA

Abstract. To understand how compensation errors occur in a nuclear data adjustment mostly devoted to U-Pu fuelled fast critical experiments and with only limited information on U-235 data, a stress test on $^{235}\text{U}(n,f)$ was suggested, using critical benchmarks sensitive to $^{235}\text{U}(n,f)$ in 1~10 keV region. The adjustment benchmark exercise with 20 integral data suggested by the NEA WPEC/SG33 was used as the reference, where practically only one experiment did give information on U-235 data. The $k_{\text{eff}}$ of HCl4.1 and HCl6.2 experimental benchmarks were used as the 21st and 22nd integral data separately to perform stress tests. The adjusted integral values and cross sections based on 20, 21 and 22 integral data using the same nuclear data and covariance data sets were compared. The results confirm that compensation errors can be created by missing essential constraints.

1. Introduction

According to the study of the NEA WPEC (Working Party on International Nuclear Data Evaluation Cooperation) /SG26 [1], a strategy of combined use of integral and differential measurements should be pursued to meet the accuracy requirements of nuclear data for Gen-IV innovative systems. The Subgroup SG33 had accomplished a study on “Methods and issues for the combined use of integral experiments and covariance data” [2], which was mainly devoted to the study of the methods of nuclear data adjustment. After that, a further topic “Methods and approaches to provide feedback from nuclear and covariance data adjustment for improvement of nuclear data files” has been studied in SG39 since 2013. It was noticed that some adjusted integral results after adjustment get worse, which was suspected to be caused by compensations in the adjustments. To prove this hypothesis and to understand how compensation errors occur in a nuclear data adjustment mostly devoted to U-Pu fuelled fast critical experiments and with only limited information on U-235 data, a stress test on $^{235}\text{U}(n,f)$ was suggested. In this test, two additional benchmarks with inter-mediate energy spectrum were added to extend the benchmark exercises of SG33 and to study the influence of changing constraint conditions in the adjustment.

2. Review of SG33 benchmark results

The brief information of nuclear data adjustment exercises of SG33 is listed in Table 1. Figure 1 give the comparison of integral parameters before and after adjustment. The results labeled as JAEA were calculated by JAEA based on JENDL-4.0 [3] and the one labeled as CIAE were calculated by CIAE with the nuclear data adjustment code NDAC [4] and the same set of nuclear data. Though all the $k_{\text{eff}}$ values had been improved after adjustment, 3 posterior spectral indices in Fig. 1, F49/F25 of ZPR6-7, F28/F25 and F49/F25 of ZPPR-9, turned worse. And after adjustment, the posterior $^{235}\text{U}(n,f)$ cross section in 1~10 keV increased by 1%.

If we look into the sensitivity coefficients of these integral parameters to $^{235}\text{U}(n,f)$ cross section, as shown in Fig. 2 and Fig. 3, we can notice that the calculated spectra index ZPPR-9 F28/F25, which has larger bias before adjustment than the former three indices in Fig. 1, have strong sensitivity to $^{235}\text{U}(n,f)$ cross section in several keV region. The former three spectral indices also have similar sensitivities. Since no other $k_{\text{eff}}$ value except that of JOYO MK-I is sensitive to $^{235}\text{U}(n,f)$ cross section in several keV region, the decrease of the all four spectral indices was thought to be driven by the eliminating of large bias of ZPPR-9 F28/F25. The increase of $^{235}\text{U}(n,f)$ cross section in 1~10 keV was probably the result of compensation effects due to the absence of essential constraints for $^{235}\text{U}(n,f)$ cross section in keV region.

3. Method of stress test

To prove the above hypothesis and to understand how compensation errors occur, a stress test on $^{235}\text{U}(n,f)$ cross section was designed.

3.1. Selection of integral experiments

The selection of fast neutron spectrum integral experiments for stress test has been based both on the magnitude of sensitivity coefficients of specific critical mass experiments to $^{235}\text{U}(n,f)$ cross sections in the 1 ~ 10 keV energy region and on the simplicity of the chosen new benchmarks simulation. Two criticality benchmarks HEU-COMP-INTER-004-001 (HCl4.1) and
Table 1. Benchmark input for adjustment exercises of SG33.

| 7 Benchmark | JEZEBEL, JEZEBEL240, FLATTOP-Pu, ZPR6-7 ST, ZPR6-7 240, ZPR9-9, JOYO MK-I |
|-------------|-------------------------------------------------------------------------|
| 11 Isotope  | B, O, Na, Cr, Fe, Ni, U, Pu |
| 8 Reaction  | (n, el), (n, inl), (n, disappearance), (n, f), Nu-total, Mu, Nu-delay |
| 20 Integral parameter | JEZEBEL-Pu 239 (k_{eff}, F28/F25, F49/F25, F37/F25), -Pu 240 (k_{eff}), FLATTOP-Pu (k_{eff}, F28/F25, F37/F25, ZPR 6/7 (k_{eff}, F28/F25, F49/F25, C28/F25), -High Pu 240 (k_{eff}), ZPR9-9 (k_{eff}, F28/F25, F49/F25, C28/F25, Na void reactivity (Step 3, 5), JOYO Mk-I (k_{eff}) |

Figure 1. Comparison of spectral indices and reactivity coefficients before and after adjustment.

Figure 2. Sensitivities of k_{eff} values to $^{235}$U(n,f) cross section.

3.2. Configuration for stress test

Three configurations for the stress test were organized based on SG33 benchmark and on the 2 additional benchmarks previously described. The original SG33 benchmarks were referred as case A(20p). For case B(21p), with the same isotopes, reactions and covariances as case A, the k_{eff} value of HCI4.1 was added as a new integral parameter. For case C(22p), the k_{eff} value of HM16.2 was added to case B. For both case B and C, the correlation coefficients between new added integral parameters and the others are assumed to be zero. In the test, nuclear data and covariances of JENDL-4.0 were used.

4. Results and discussion

4.1. Test1: Case A (20p) vs. case B (21p)

Different constraint conditions can lead to different direction of adjustments for integral parameters. Figure 4 gives the variation of integral parameters after adjustment for case A and B. When comparing the integral parameters after adjustment for case A and for case B, the improvement of k_{eff} values for HCI4.1 was added as a new integral parameter. For case C(22p), the k_{eff} value of HM16.2 was added to case B. For both case B and C, the correlation coefficients between new added integral parameters and the others are assumed to be zero. In the test, nuclear data and covariances of JENDL-4.0 were used.

Different constraint conditions can also lead to opposite directions of cross section adjustments. Figure 5 shows the comparison of the relative variation of cross sections among cases A, B and C. To improve the calculated k_{eff} for HCI4.1, the posterior $^{235}$U(n,f) cross sections obtained in case B were decreased by 5% from $^{235}$U fission in 1~10 keV region have been selected from ICSBEP2006 [4]. HCI4.1 is a k_{sc} experiment with intermediate spectrum. The benchmark model is an infinity HEU moderated by graphite. This experiment was design to provide a sensitivity test of $^{235}$U cross section over the energy range 10 eV to 10 keV. HM16.2 is also an intermediate-spectrum critical assembly, with a graphite-HEU core surrounded by a copper reflector. The sensitivity coefficients for k_{eff} of HCI4.1 and HM16.2 are compared to those for the SG33 benchmarks in Fig. 2. The sums of the sensitivity coefficients from 1~10 keV for HCI4.1 and HM16.2 are more than 3 times larger than that for JOYO MK-I.
Figure 4. Comparison of integral parameters before and after adjustment for case A and B.

0.4 to 2 keV and decreased by 2% from 2 to 10 keV instead of a systematic increase obtained in case A. On the contrary, $^{235}$U(n, disappearance) cross sections from 0.7 to 2 keV were increased in B but decreased in A; and $^{10}$B(n,α) cross section was also increased 0.1 ∼ 0.6% < 1 MeV. Although the adjusted SVR of ZPFR-9 did not change from A to B, the influence of $^{235}$U(n,f) cross section decrease in the keV energy region was compensated by the increase of $^{23}$Na(n,el) cross section in keV energy region.

4.2. Test2: Case A vs. case B vs. case C (22p)

In test2, different constraint conditions lead to different posterior integral parameters again. Figure 6 gives the variation of integral parameters after adjustment for case A, B and C. When comparing the apriori and posterior integral parameters for A, B and C, the posterior $k_{eff}$ values for SG33 benchmarks are almost the same, but the posterior $k_{eff}$ of HCI4.1 for case C get worse than in case B. The posterior spectral indices values for ZRP6-7 ST and ZRRP-9 of C are between the A and B posterior values. The requirement to account for the small uncertainties of the $k_{eff}$ value of HMI6.2 caused the variations of the of integral parameters values from case B to C.

The posterior cross sections also changed significantly from case B to C, as shown in Fig. 5. To improve the $k_{eff}$ of HCI4.1 and HMI6.2 simultaneously, the $^{235}$U (n,f) cross sections in case C were decreased by 4% in 0.4 ∼ 2 keV region but increased by 1% in 3 ∼ 10 keV region, which is in partial agreement with that of case B. The $^{235}$U (n, disappearance) cross sections from 0.4 to 2 keV in case C were decreased by 4% instead of the increase by 5% in B. To still improve the prediction of $k_{eff}$ value for HCI4.1 in case C, the $^{10}$B(n, disappearance) cross sections below 20 keV have been further increased to compensate the increase of $^{235}$U(n,f) cross section. Since the increment of $^{235}$U(n,f) cross section in case C is no longer as large as in case B, the $^{23}$Na(n,el) cross section is also no longer increased as much as in case B. This confirms that different constraint conditions always give different posterior nuclear data and different compensation effects.
In the current stress test, not only cross sections but also ratios of cross sections change significantly from case to case, since no differential experiment information on the $\alpha$ value of $^{235}$U was included in the adjustment. As shown in Fig. 7, the $\alpha$ value of $^{235}$U in 1–2 keV energy region increases by 10%, that did help to improve the prediction of the $k_{\text{eff}}$ value of HCl4.1. However, this effect in keV region was partially eliminated by the need of maintaining a good prediction of the $k_{\text{eff}}$ value of HM16.2 in case C. Moreover, to improve the prediction of HM16.2, more than 20% decrease of $\alpha$ value and capture cross sections between 3.6–6 MeV (as shown in in Fig. 5 and Fig. 6) were also needed, in order to compensate the decrease of $^{235}$U(n,f) cross section in keV region. That means that compensation effects occurs not only among different isotopes and reactions, but also that they do occur in different energy regions.

5. Summary
To understand how compensation effects can arise in nuclear data adjustments based on the General Least Square method, a stress test on $^{235}$U(n,f) cross sections has been performed using U-Pu fuelled fast critical experiments together with a set of integral benchmark information specifically sensitive to U-235 data. The test results show that the posterior of integral and differential changes from case to case when input integral information changes.

We can conclude that different constraint conditions will give different, even opposite posterior results both for integral and differential data as a result of a nuclear data adjustment. Compensation effects are almost unavoidable in the adjustment of different isotopes and reactions, in different energy regions. Missing essential constraints will most probably lead to compensation errors. To avoid compensation error and generate adjusted nuclear data library for general purpose, we have to construct complete constraint conditions. Even to obtain a special purpose library, input information has to be carefully prepared. New approaches have been proposed to avoid as much as possible compensations and some discussion will be made in a companion paper at this Conference [6].

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