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New ^{23}Na evaluation in the resolved resonance range taking into account both differential and double differential experiments

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Abstract. In 2012 CEA produced a entire new evaluation of sodium nuclear data for the release of the JEFF-3.2 evaluated nuclear data library. During the evaluation process performed with the CONRAD code, several differential measurements (total and discrete inelastic cross-sections) have been used. However double differential data (elastic angular distribution) that were yet available in the EXFOR database were not incorporated in the analysis at that time. The experimental elastic angular distribution were discarded because of it was impossible to obtain a good agreement for both angle-integrated cross-sections and double differential ones. The underlying cause of this disagreement is expected to be due to the attribution of quantum numbers to resonance and related channel amplitudes. Indeed these numbers are imposed during the analysis but impact differently angular distributions and angle-integrated cross-sections. An automated search for an accurate set of quantum numbers has been implemented in order to produce a reliable quantum numbers set. In this paper we present a new evaluation of Na-23 taking into account both differential and double differential measurements. The analysis performed with the CONRAD code reached the level of agreement with experimental data for the total and inelastic cross-sections but this time with a significant improvement for the elastic angular distributions. This new evaluation produced in the ENDF-6 format has then been tested and validated on critical facilities calculation (MASURCA and ZPPR) in different configurations (nominal and voided) in order to assess its performances.

1 Introduction

In 2012, the nuclear data team at CEA-Cadarache produced an ^{23}Na evaluation for the release of the JEFF-3.2 library [1]. This new evaluation was based on several angle-integrated differential (energy-dependent) experiments (for the total and discrete inelastic channels), however double differential (energy- and angle-dependent) experiments such as Kinneys angular elastic cross-section measurements [2] were not taken into account at that time. The main difficulty was to achieve a good agreement on both angle-integrated cross-sections and double differential ones. We present here investigation work on the ^{23}Na evaluated data. This paper focuses on the resonance energy range, where the impact of the resonance quantum numbers on the angular differential data has been studied. A new set of resonance parameters have been produced and tested on a set of sodium void benchmarks that are particularly sensitive to ^{23}Na nuclear data. We also shows that all experimental conditions must be included in the analysis, namely the Doppler-broadening and the resolution function. Additionally we attempted to change the usual boundary conditions convention from $B_c = S_c$ to $B_c = -\ell$ as recommended in Ref. [3], S_c being the usual energy-dependent *shift-factor* of the R-matrix theory [4].

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2 Status of the JEFF-3.2 ^{23}Na evaluation

The latest evaluation of ^{23}Na relied on a set of experimental data, for the resonance resonance range the following data were considered

1. Larson 1976 total cross section measurement [5] which covers the range [32.479 keV; 37.399 MeV]
2. Rahn 1965 total cross section measurement [6] which covers the range [87.6 eV; 318.7275 keV]
3. Kinney 1976 angular elastic cross section measurement [2] which covers the range [550 keV; 2 MeV]
4. Rouki 2012 inelastic cross section measurements [7] for the first six levels which covers the range [459.41 keV; 3.8264 MeV]

We note that other good-resolution data are also available, namely the angular elastic cross section [8] from Kopecky (1997) but that are believed to require a special angular-dependent multiple scattering correction, which is currently unavailable in the CONRAD code [9] used for the present work.

The major identified defect of the JEFF-3.2 ^{23}Na evaluation lays in elastic scattering angular distribution. Indeed although some experimental data were available in 2012, elastic scattering angular cross section measured by Kinney [2] in 1976 were not incorporated in the analysis. This lack of experimental constraints could lead to a misassignment of the resonance quantum numbers J^π, ℓ, s. Therefore even though angle-integrated cross section were in a reasonable agreement with experimental data, the angular-differential cross sections were incorrect, especially in the backward direction. In the present work we have included the Kinney data and made an automatic search for the resonance quantum numbers. This procedure improved strongly the agreement with angular distributions (see Fig. 1) while keeping a good agreement with integrated data. We can see in Fig. 1 that the agreement is still not perfect meaning that either a deeper investigation should be carried out (for instance allowing several neutron channels for each resonance), or that the model may be improved as explained in Sec 4.

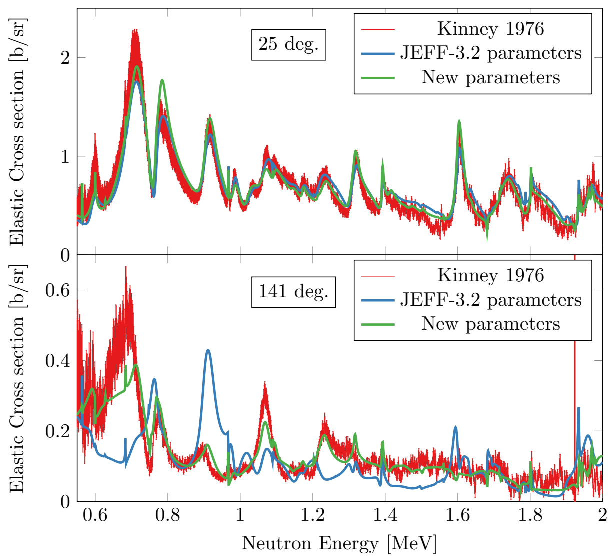

Figure 1. Angular elastic cross sections obtained with the JEFF-3.2 resonance parameter set and with the new set obtained after re-attributing resonance quantum numbers.

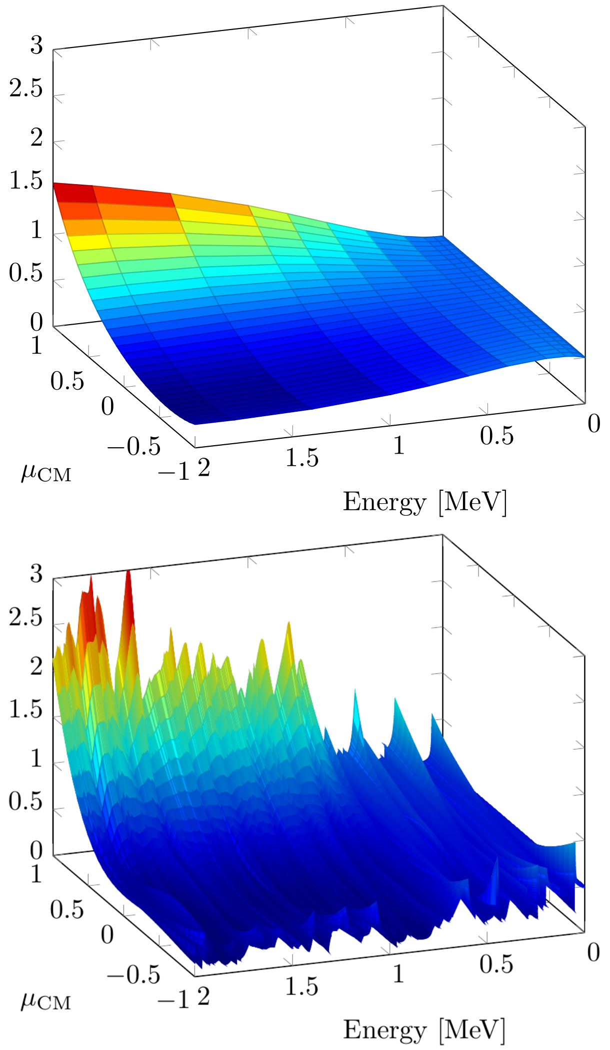

Figure 2. Elastic angular distribution of ^{23}Na in the JEFF-3.2 evaluation file (above) and in the present work (below).

Now that we expect a better agreement between experimental data and angular cross section obtained for the new set of resonance parameters, we produced and processed a new ENDF-6 file mostly based on JEFF-3.2 but in which the resonance parameters have been replaced as well as the angular distribution. The former angular distribution present in JEFF-3.2 were produced using the TALYS reaction code [10] that uses statistical models. Therefore the resonant structure observed in the resolved resonance range in the angular distribution were not present in the JEFF-3.2 evaluation, as shown in Fig. 2. With our new file the angular distribution exhibit resonant structures consistent with the model used for the modeling of angle-integrated cross sections. This consistency was already present in the ENDF/B-VII ^{23}Na evaluation but was one of the defect of the JEFF-3.2 one.

3 Benchmarking the evaluation

Having obtained a new set of resonance parameters, the new evaluated data have been tested on a set of integral benchmarks known to be highly sensitive to ^{23}Na data. These are the ZPPR-10A sodium void effect described in the IRPhEP database [11] (see Fig. 4) and the Racine and Pre-Racine (see Fig. 3) sodium void effect measurements performed at the MASURCA facility at CEA/Cadarache [12, 13].

The C/E results for these benchmarks are shown in Tab. 1, it can be observed that the new evaluation of the sodium resonances improve significantly the global trend of JEFF-3.2 that overestimates the void effect.

4 Remaining open issues

While working on the Larson data we realized that some small resonances are impacted by the energy resolution and Doppler-broadening. These experimental conditions were not considered in the previous work that led to JEFF-3.2. Indeed for light isotopes with large resonant structure one expect that the Doppler-broadening has a limited impact. Additionally, when working with high-resolution experimental data, typically obtained with a long flight-path one also expect that their is no need to use a resolution

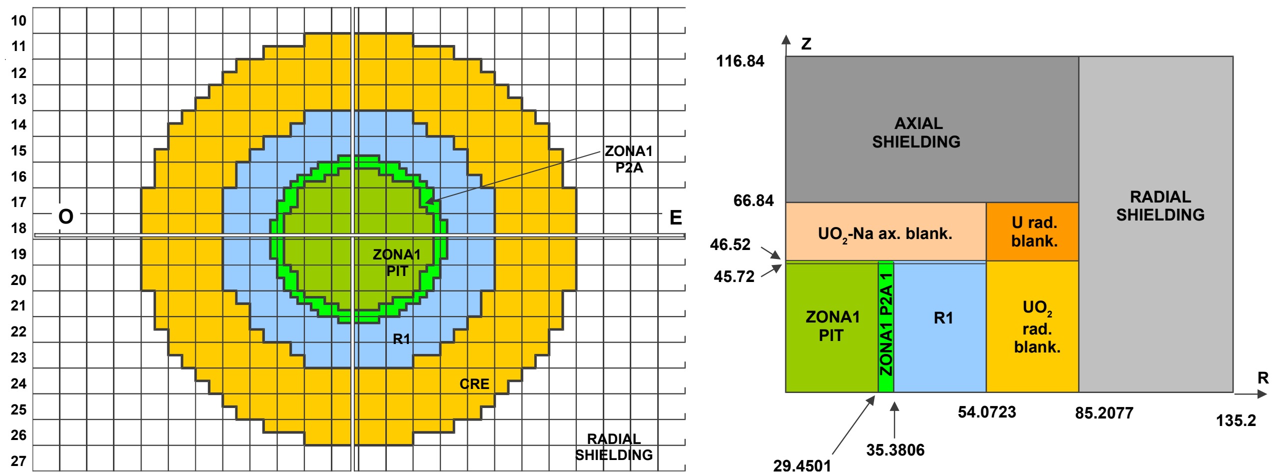

Figure 3. XY layer and RZ representation of the PRE-RACINE-2B experiment [12, 13] taken from Ref. [14].

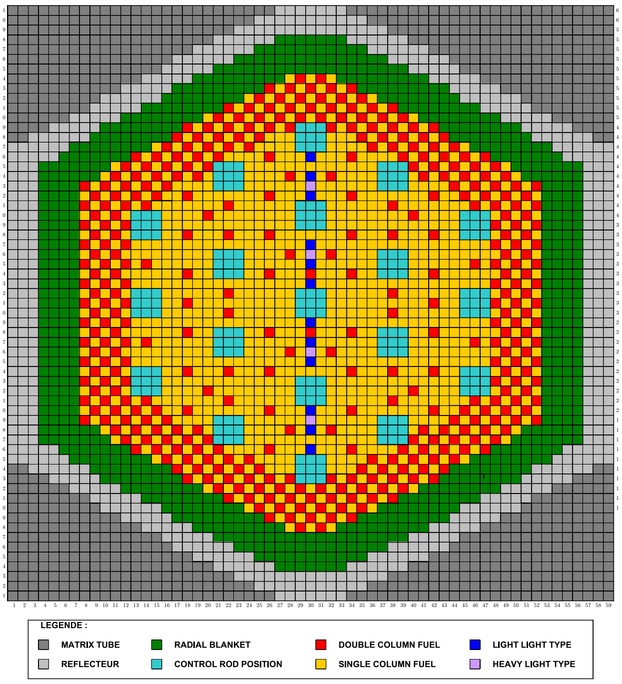

Figure 4. XY view of the ZPPR-10A core [11] taken from Ref. [14].

function to analyze the data. We tested these hypotheses on the Larson data with a 300 K Doppler broadening and for which the reported [5] energy resolution is

$$\left(\frac{\Delta E}{E}\right)^2 = [0.19 + 0.42E(\mathrm{MeV})] \times 10^{-6} \quad (1)$$

It was found that these experimental conditions impact the narrow resonances as illustrated in Fig. 5 where the Doppler broadening (Dop.) the the energy resolution function (RF) are successively added.

In the JEFF-3.2, the ENDF convention for the choice of boundary condition parameter [4] $B_c = S_c(E)$ was applied. However this choice is justified mainly for neutron-induced reactions on actinides for which $\ell = 0$ implies

Table 1. Benchmark results for the JEFF-3.2 and the new resonance parameters set on integral sodium void effect experiments.

Experiment	C-E JEFF-3.2	C-E new eval.	Exp. unc.
ZPPR-10A void 4	9.4 ± 2.3	-1.0 ± 2.0	1.7
ZPPR-10A void 6	10.1 ± 1.8	-4.4 ± 1.9	2.3
ZPPR-10A void 8	5.2 ± 1.8	-3.2 ± 2.1	2.1
ZPPR-10A void 9	9.5 ± 3.5	-2.5 ± 2.6	1.9
Pre-Racine 2B void 5	80.7 ± 2.6	67.9 ± 2.5	8
Racine 1A void 4	20.7 ± 2.5	5.1 ± 2.3	9
Racine 1A void 10	11.9 ± 2.3	3.5 ± 2.3	8
Racine 1D void 2	28.8 ± 2.3	20.5 ± 2.3	5

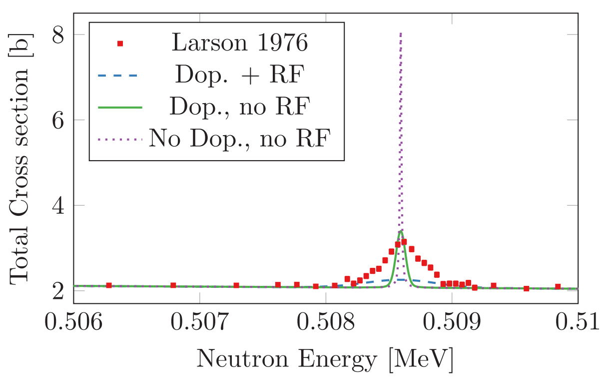

Figure 5. Illustration of the impact of the consideration of the sample temperature and the energy resolution in the Larson total cross section measurement for the narrow resonance near 509 keV.

$B_c = 0$. Indeed in a rigorous implementation of the R-matrix theory, the boundary condition B_c must be energy-independent, ensuring that the many-body nucleus wave function can be properly expanded on eigen functions. In the case of ^{23}Na, many resonance are attributed quantum numbers with $\ell > 0$, therefore the usual ENDF convention is not justified. To investigate the possible impact of this $B_c = S_c(E)$ we restarted "from scratch" a new resonance range analysis starting from 0 eV to 700 keV with the boundary condition choice $B_c = -\ell$. With this new boundary condition choice, the eigen energies E_λ do not correspond anymore to the observed resonance energies. Finding good initial guess of the resonance parameters becomes very tedious therefore we limit the analysis below 700 keV. The first results of this attempt are shown in Tab. 2 where the χ^2 for all listed experiments are given. The results obtained with the new boundary choice $B_c = -\ell$ seem better on average than those obtained with either the JEFF-3.2 or the new resonance parameters set presented here. In particular it seems to improve even further the angular distribution at forward angles. It must be kept in mind that these results are not directly comparable as for obtaining the resonance parameters for JEFF-3.2 or for the new evaluation, the inelastic cross section measurement of Rouki [7] was also included whereas it was not for the set with $B_c = -\ell$. In future we plan to extend this work by using the alternative Brune parameterization [15] which allows to work back with eigen energy parameters that matches the resonance energies but with a consistent boundary condition choice. This parameterization would allow to extend our analysis range and confirm whether improvements are truly expected for angular distributions.

Table 2. Agreement between presented resonance parameters sets and Larson (total cross section) and Kinney (elastic angular cross section) experimental data.

Experiment	JEFF-3.2	new Eval.	$B_c = -\ell$
Larson	6610	3112	1618
Kinney 25deg	212	124	128
Kinney 40deg	57	88	62
Kinney 57deg	95	73	39
Kinney 92deg	1117	348	218
Kinney 127deg	1056	84	119
Kinney 141deg	1568	268	138
Kinney 156deg	246	583	205

5 Conclusion

We showed here that a new evaluation of the ^{23}Na resonance parameter considering differential and angular-integrated experimental cross sections can lead to a significant improvement of the C/E agreement in integral void effect benchmarks. However in our analysis we saw that some remaining issues still need to be addressed for instance the use of a more physical boundary condition $B_c \neq S_c(E)$ or the inclusion of the experimental conditions such as the Doppler-broadening and the consideration of the energy-resolution of the experimental data. More comprehensive analysis work is planned in near future.

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