RESONANCE REGION EVALUATION OF ^{16}O FOR CRITICALITY SAFETY AND REACTOR APPLICATIONS

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Abstract. The intent of this paper is to present the resolved resonance evaluation of ^{16}O in the energy range from thermal to 6 MeV. The newness of the present work is that recent cross-section data for the ^{16}O(n,α)^{13}C reaction taken at the GELINA time-of-flight facility and transmission data obtained at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR) were included in the evaluation. The evaluation was carried out with the SAMMY code. The evaluation was used to calculate critical benchmark experiment sensitive to the ^{16}O cross sections.

1 Introduction

Normalization issues of existing ^{16}O(n,α)^{13}C reaction cross section have generated renewed interest on measuring the (n,α) cross section data. The Nuclear Energy Agency High Priority Nuclear Data Request List demonstrate the interest on accurate ^{16}O(n,α) cross-section data for practical applications.[1] Recent experimental data measurements, namely transmission and (n,α), have motivated revising the ^{16}O resonance region evaluation. Issues with the normalization of the (n, α) cross sections have been investigated and a very dependable measurement has been carried out at the GELINA facility at the Joint Research Center (JRC) Geel from the energy threshold 2.354 MeV to 9 MeV. Additionally, transmission measurements were done at the nELBE time-of-flight (TOF) facility at Helmholtz-Zentrum Dresden - Rossendorf (HZDR). Experimental data used in previous evaluations were also considered in the evaluation. The resonance evaluation was performed in the energy range from 0 eV to 6 MeV using the reduced R-matrix Reich-Moore methodology of the computer code SAMMY resulting in a set of resonance parameters (RPs) that describes well the experimental data used in the evaluation. The recent transmission measurements and the (n,α) cross section data are well reproduced. The RPs were converted to the evaluated nuclear data file (ENDF) format using the R-Matrix Limited format option LRF=7 that allows adding information that could not be accommodated in other ENDF representation of RPs. The intent of the paper is to describe the procedures used in the evaluation of the RPs and the use of the RPs in calculations of critical benchmark experiments. Preliminary results for Pu-SOL-THERM-041 (PST-041) configurations listed in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook indicates an improvement on the average k_{eff} values with calculated k_{eff} being consistent with the benchmark k_{eff}, discrepancies on k_{eff} not exceeding the combined effect of experimental and Monte Carlo uncertainties. The PST benchmark consists of series of 40 experiments carried out at the Valduc research center in response to criticality safety needs. In particular, for the PST-041 series the changes in k_{eff} values indicate that these benchmarks are sensitive to the (n,α) cross section of ^{16}O and that the new measurements were essential to improve the benchmark results.

2 RESONANCE EVALUATION OF ^{16}O FROM THERMAL TO 6 MEV

2.1 Experimental data

Resolved resonance evaluation of ^{16}O cross section using the code SAMMY [2] in the energy range from thermal to 6 MeV has been reported in Reference [3] which addresses concerns with regard thermal capture and scattering cross section data, coherent scattering data and present an attempt to quantify the normalization issue in connection to the (n,α) cross section. Two sets of resonance parameters, named low and high, from which the calculated (n,α) cross sections differed by ~30 %. From these sets of resonance parameters benchmark calculations of systems sensitive to the (n,α) cross section were carried out. Improvements on the k_{eff}, in comparison with results of (n,α) cross section evaluation available in the ENDF/B-VII.1 are observed with a better performance to the set of resonances named low. After the study presented in Reference [3], there had been attempt to unveil the normalization (n,α) cross section issue. As a result, measurements of (n,α) cross section were done at the time-of-flight (TOF) GELINA facility at the JRC from the energy threshold 2.354 MeV to 9 MeV [4]. In addition, transmission measurements at the nELBE TOF facility at HZDR were also done in the energy range 100 keV to 10 MeV.[5] The experimental data sets used in the SAMMY evaluation process are displayed in Table 1. Listed in Table 1 are the experimental data used in Reference [3] and the somehow recent (n,α) cross section measurements performed at GELINA and nELBE.

Table 1. Experimental data for the ^{16}O evaluation.

Data	TOF (m)	Energy range (MeV)	Reference	Date
Capture cross section	-	Thermal	Firestone [7]	2015
Coherent scatterin g length	-	-	Sears [8]	1992
Total cross section	79.46	2.0-6.3	ORELA [9, 10]	1980
Total cross section	249.75	2.0-6.3	RPI [11]	2015
Total cross section	41.0 and 47.0	0.6–4.3	ORNL Van de Graaff [12]	1973
Total cross section	189.25	3.14–6.3	KFK cyclotron [13]	1980
(n,α) extracted from (α,n)	-	3.2–6.3	ORNL Van de Graaff [14]	1973
(n,α) extracted from (α,n)	-	3.0–6.3	Tandem Accelerator Universtät Bochum [15]	2005
(n,α) measure ments	60	2.354–9.0	GELINA [4]	2020
Transmis sion	9.18	0.1–10.0	nELBE [5]	2020

2.2 Data evaluation

The experimental data indicated in Table 1 were evaluated with the SAMMY code, and in addition to the RPs resonance parameter also covariance (RPCs) were also derived. Up to the (n,α) energy threshold (2.354 MeV) each resonance level is represented by the energy of the resonance E_r, gamma width Γ_γ, and the neutron width Γ_n. Above the threshold an additional channel to represent the (n,α) reaction is added to each energy level with the width Γ_α. The experimental data are well represented with the RPs in conjunction with the reduced R-matrix Reich–Moore formalism. The RPs resulting from the evaluation include 54 resonances with 3 energy bound levels and 16 resonance levels above 6 MeV. Capture and scattering cross sections at thermal (0.0253 eV) obtained with calculation using the evaluated resonance parameters are listed in Table 2. Also included in Table 2 are the capture resonance integral and the coherent scattering length. The calculated values listed in the Atlas of Neutron Resonances (ANR) [6] are also listed in Table 2. The quantities listed in Table 2 are the thermal capture and scattering cross sections $\boldsymbol{\sigma}_\gamma$, and $\boldsymbol{\sigma}_s$, the coherent scattering length a_{coh}, and the capture resonance integral I_γ, which is defined as integral from 0.5 eV to 20 MeV with a $1/_E$ weighting spectrum. One caveat regarding the ANR scattering cross section is that it is related to the value calculated at the 0 K temperature. The value calculated with the RP at 0 K is 3.765 ± 0.025 b. The uncertainties included in the values calculated based on the RP are that generated with RPC. The good agreement between the coherent scattering derived with the resonance parameters with experimental values is the result of a careful determination of the energy bound levels. They were determined according to the excitation energy levels of the compound nucleus ^{17}O, that is the n+^{16}O interaction. The SAMMY fitting of four experimental data displayed in Table 1 is shown in Fig. 1.

Table 2. Values at thermal (0.0253 eV)

Quantity	Experimental [7, 8]	ANR [6]	Evaluation T = 293.6 K
$\boldsymbol{\sigma}_\gamma$ (barns)	(1.67 ± 0.023) × 10^{-4}	(1.9 ± 0.19) × 10^{-4}	(1.67 ± 0.03) × 10^{-4}
$\boldsymbol{\sigma}_s$ (barns)	-	3.761 ± 0.006	3.884 ± 0.022
a_{coh} (fm)	5.803 ± 0.004	5.805 ± 0.005	5.801 ± 0.005
I_γ (barns)	-	(2.7 ± 0.3) × 10^{-4}	(3.09 ± 0.42) × 10^{-4}

Two transmission data are displayed in Fig. 1, namely the data taken at GAERTTNER RPI linear accelerator (the very bottom picture), the most recent transmission data taken at the German laboratory nELBE. The (n,α) data are the Harissopulos data with a 30 % normalization and the data taken at GELINA by Urlass. The SAMMY fitting of the data shown in Table 2 provided a reasonable χ^2 and an average of experimental-to-fitting residual of about 0.8 %. The Urlass data agrees well with the Harissopulos data normalized to 30 %.

It should be mentioned that the resonance parameters are also used to generate angular dependent cross section data as well as data uncertainties calculated with the resonance parameters covariance.

3 Benchmark results

The ^{16}O evaluation presented in this paper has been used for benchmark calculations of systems sensitive to the ^{16}O cross section data. The results are for the Pu-SOL-THERM-041 (PST-041) benchmark configurations listed in the International Criticality Safety Benchmark

Evaluation Project (ICSBEP) handbook.[16] This series of 40 experiments performed at Valduc research center involves solutions of low ^{240}Pu content (3 %) plutonium nitrate with a concentration in plutonium varying between 20 g/L and 190 g/L, in a 500 mm/200 mm annular tank.

Criticality calculations, k_{eff}, were performed using the MORET 5 Monte Carlo transport code [17] and various nuclear data libraries (JEFF-3.1.1, JEFF-3.3, JEFF-4T1, ENDF/B-VII.1, ENDF/B-VIII.0 and JENDL-4.0) with a low Monte Carlo uncertainty of 10 pcm (±0.00010). Only results for the JEFF-4T1 library are reported in this paper. The impact of the new oxygen evaluation was tested by including the new oxygen evaluation in the JEFF-4T1 library. The characteristics of the benchmark cases along with the k_{eff} results are reported in Table 3. Figure 2 also plots the k_{eff} results versus the energy corresponding to average lethargy of neutrons causing fission (EALF). The experimental uncertainty at the 1σ level is indicated using red dotted lines.

The comparison of JEFF-4T1 results with those where oxygen is replaced by the old evaluation in JEFF-4T1 library indicates an improvement on the average k_{eff} values. Indeed, calculated k_{eff} are more consistent with the benchmark k_{eff}, since the differences on k_{eff} do not exceed the combined effect of experimental and Monte Carlo uncertainties.

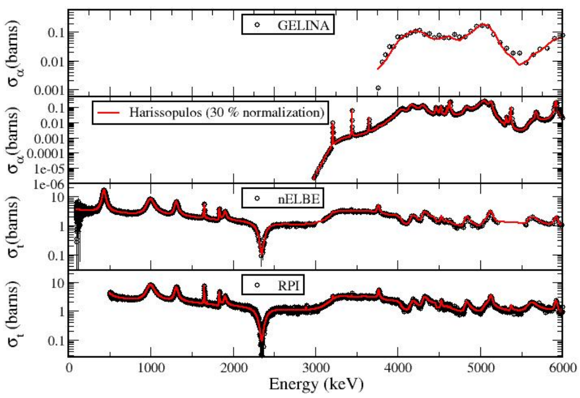

Fig. 1. Fitting of the experimental data up to 6 MeV with SAMMY.

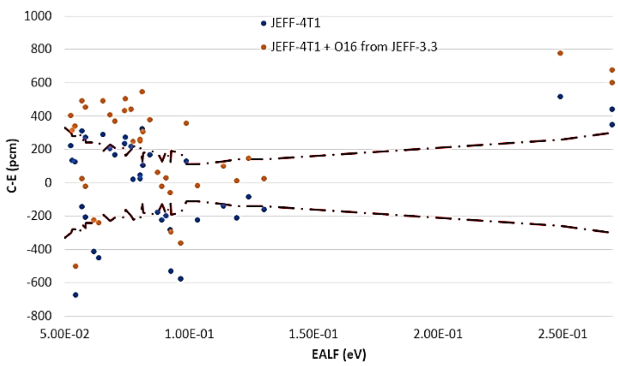

Fig. 2. k_{eff} results for PST-041 versus EALF (eV).

4 Conclusions

This paper presents a new ^{16}O resolved resonance evaluation in the energy range from thermal to 6 MeV using the Reich-Moore approach of the SAMMY code. Recent transmission and (n,α) cross section data were included in the evaluation together with data used in previous evaluation. The resulting set of resonance parameters reproduces the experimental data very well. The impact of using the new evaluation on benchmark calculations has been verified for critical benchmark systems sensitive to ^{16}O. It is a series of 40 ICSBEP plutonium solution benchmark. The results of using the new evaluation show that the average k_{eff} obtained with calculations using JEFF4T1 with the new ^{16}O evaluation and with a ^{16}O evaluation included in JEFF3.3 differs of about 200 pcm favouring the new evaluation.

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Table 3. Characteristics of PST-041 cases and k_{eff} results (σ_{MC} = 0.00010).

Benchmark	**EALF (eV)**	**C(Pu) g/L**	**^{240}Pu %**	**k_{eff} JEFF-4T1**	**k_{eff} JEFF-4T1 + O^{16} from JEFF-3.3**
PST-041-001	9.28E-02	65.9	3.11	0.99468	0.99703
PST-041-002	9.67E-02	65.9	3.11	0.99422	0.99637
PST-041-003	9.07E-02	61.35	3.11	0.99800	1.00029
PST-041-004	8.73E-02	61.35	3.11	0.99823	1.00063
PST-041-005	8.44E-02	55.8	3	1.00165	1.00378
PST-041-006	8.14E-02	55.8	3	1.00102	1.00305
PST-041-007	8.03E-02	51.65	3.11	1.00044	1.00257
PST-041-008	8.03E-02	51.65	3	1.00025	1.00249
PST-041-009	7.76E-02	51.65	3.11	1.00020	1.00244
PST-041-010	7.41E-02	48	3	1.00234	1.00431
PST-041-011	7.65E-02	48	3	1.00215	1.00439
PST-041-012	7.03E-02	41.3	3.11	1.00165	1.00367
PST-041-013	6.82E-02	41.3	3	1.00202	1.00407
PST-041-014	6.36E-02	33.74	3	0.99549	0.99760
PST-041-015	6.19E-02	33.74	3	0.99584	0.99777
PST-041-016	5.85E-02	28.1	3.11	0.99790	0.99978
PST-041-017	5.70E-02	28.1	3	0.99853	1.00022
PST-041-018	5.45E-02	23.5	3	0.99325	0.99497
PST-041-019	1.30E-01	100.46	3	0.99839	1.00023
PST-041-020	1.24E-01	100.46	3	0.99913	1.00146
PST-041-021	1.19E-01	91.05	3.11	0.99789	1.00012
PST-041-022	1.14E-01	91.05	3	0.99861	1.00098
PST-041-023	1.03E-01	76.81	3	0.99774	0.99979
PST-041-024	9.89E-02	76.81	3	1.00127	1.00355
PST-041-025	8.90E-02	66.22	3.11	0.99775	0.99975
PST-041-026	9.23E-02	66.22	3	0.99715	0.99939
PST-041-027	8.12E-02	55.08	3.11	1.00320	1.00546
PST-041-028	7.45E-02	50.5	2.99	1.00272	1.00502
PST-041-029	6.54E-02	40.15	2.99	1.00286	1.00491
PST-041-031	5.85E-02	30.25	3.11	1.00272	1.00451
PST-041-032	5.71E-02	30.25	3.11	1.00309	1.00490
PST-041-033	5.30E-02	25.1	3.11	1.00132	1.00312
PST-041-034	5.42E-02	25.1	3.11	1.00126	1.00339
PST-041-035	5.26E-02	23.2	3.11	1.00219	1.00400
PST-041-037	5.00E-02	19.98	3.11	1.00207	1.00375
PST-041-038	2.70E-01	189.05	3.11	1.00349	1.00598
PST-041-039	2.70E-01	189.05	3.11	1.00440	1.00675
PST-041-040	2.49E-01	189.05	3.11	1.00514	1.00777
Mean k_{eff}				**1.00001**	**1.00211**