

Neutron Data Files for Pd-107, I-129 and Cs-135

YongDeok Lee and Young-Ouk Lee

Korea Atomic Energy Research Institute, P.O Box 105, Yusong, Daejeon, Korea 305-600, ydlee@kaeri.re.kr

1. Introduction

From the request of the accelerator driven system concerning the toxicity for a waste transmutation, the neutron reaction cross sections on Pd-107, I-129 and Cs-135 were considered for examination and finally re-evaluated. The current evaluation of the neutron induced cross section data was from an unresolved energy to 20 MeV. These nuclei usually have a very long half-life: I-129 has been of particular concern in nuclear reactors because of its 16 million year half-life, affinity to thyroid and volatility in the elemental state. Pd-107 has a 6.5 million year half-life and exists as a fission product poison in a fission reactor. Pd-107 exists at a 15.7 weight percent among the isotopes in a fission. Cs-135 has a 2.3 million year half-life. Pd-107, I-129 and Cs-135 nuclei have a beta particle decay and transit to Ag-107, Xe-129 and Ba-135, respectively, after being produced from the fission. In ENDF/B-VI, the evaluation was done in 1989, 1980 and 1998 for Pd-107, I-129 and Cs-135, respectively.

The evaluation consists of an optical model potential search followed by a complete nuclear reaction model calculation and validation with the experimental data. Nuclear reaction cross sections were calculated using the recently released Empire-II code[1]. The calculated cross sections are graphically compared with the experimental data and the evaluated files (ENDF/B-VI, JENDL-3.2, JEF-2.2, BROND-2 and CENDL-2). The evaluated results are compiled to ENDF-6 format and finally, they are merged with the resonance results to make the full data file.

The general information file (MF1) was setup for each nucleus; including an evaluation history, code utilization, evaluation procedure, tuning parameters, resonance description, reaction description and references. The new data file involves the cross sections from a thermal energy to 20 MeV and it is ready to submit to the ENDF/B-VII.

2. Model

Scat2-Empire code [1] combination was adopted in the current cross section calculation for the total, elastic scattering and reaction cross sections. The energy dependent optical model potential was decided for the fast energy range and applied for the calculation of the transmission coefficients. The discrete and continuum levels for the compound and residual nuclei were decided

as well. The individual nuclear reaction cross sections were calculated using the statistical model for the equilibrium energy region and the quantum mechanical approach for the pre-equilibrium energy region.

The code combination accounts for the major nuclear reaction mechanisms, such as the optical model, the Multistep Direct (TUL model, codes ORION & TRISTAN), the Multistep Compound (NVWY model) and the full featured Hauser-Feshbach model, including a width fluctuation correction[1]. The Multistep direct model takes care of the inelastic scattering to vibrational collective levels and the decay information. The direct-semidirect (DSD) capture model[1] was recently incorporated into the Empire to improve the fast neutron capture in the pre-equilibrium energy region. Empend in the Empire package is used to make the ENDF-6 format file.

For the level densities and discrete levels, a dynamical approach for the densities was used as parameterized by the Empire code, after a careful matching to low-lying discrete levels. Discrete levels were taken from the library built-in Empire that is based on the 1996 version of the ENSDF database. Default gamma-ray strength function was used for a capture reaction. However, it can be adjusted to fit the calculation to the experimental data.

The optical model potential form and corresponding parameters, as a function of the incident neutron energy, were searched in an optical model based on the reference experimental data. To obtain proper potential parameters, the Woods-Saxon well is used for the real part potential in the optical model:

$$V(r) = -V/(1+\exp((r-R_v)/a_v)) \quad (1)$$

where V , a_v are the strength and diffuseness of the potential, respectively. The nuclear radius R_v , related to mass number A , is given by

$$R_v = r_v A^{1/3} \quad (2)$$

For the imaginary part potential, the derivative Woods-Saxon shape is used and the Thomas form is taken in the optical model potential for a spin-orbit coupling:

3. Calculation

The data file involves the (n, tot) , (n, n) , (n, n') , $(n, 2n)$, $(n, 3n)$, $(n, n\alpha)$, (n, np) , (n, γ) , (n, p) and (n, α) cross sections. In the paper, (n, γ) cross section connected with the resonance part is shown in the figures.

Fig. 1 shows the capture cross section on Pd-107. The current evaluation and the ENDF/B-VI are in good

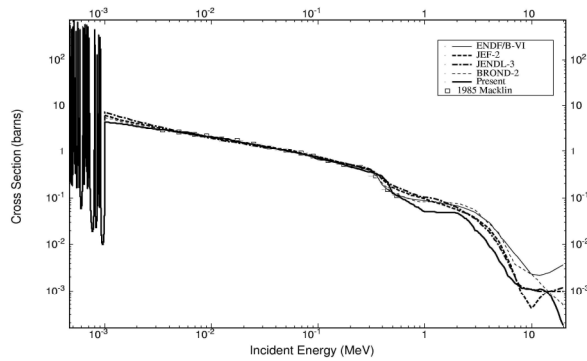


Figure 1. Capture cross section on Pd-107 (the fast energy region was merged with the resonance part).

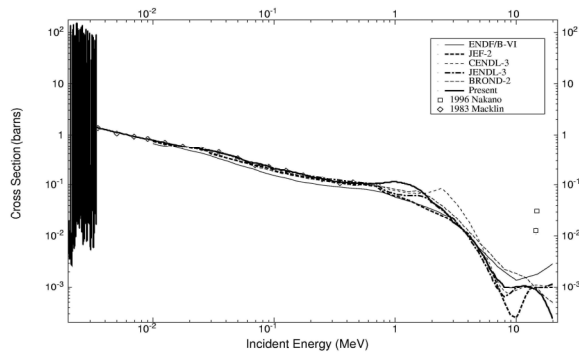


Figure 2. Capture cross section on I-129 (the fast energy region was merged with the resonance part).

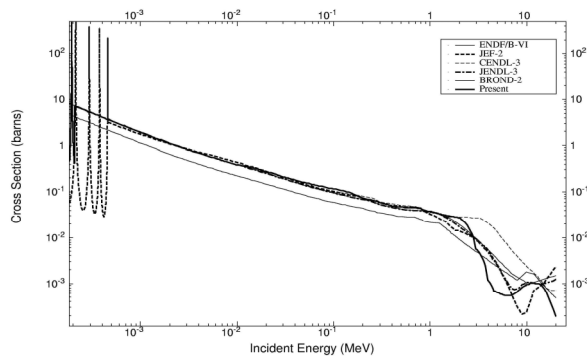


Figure 3. Capture cross section on Cs-135 (the fast energy region was merged with the resonance part).

agreement with the experimental data[2] in the measured energy region. However, above 600 keV, a discrepancy appears. In that energy range, the ENDF/B-VI is higher than the calculation. For the total and capture cases, the current file shows a continuity and a smoothness at the merge with the resonance.

Fig. 2 is the capture cross section on I-129. The calculation agrees well with the experimental data[3]. The ENDF/B-VI is just a little lower than the measured data. Fig. 3 is the capture cross section on Cs-135. The default

parameters[4] loaded by Empire were used, however, in the fast energy region, the calculation is higher than the ENDF/B-VI. Specially, around 14 MeV, the calculation shows the pre-equilibrium direct capture phenomena.

4. Conclusion

The evaluation of the selected long half-life nuclei for the waste transmutation had a difficulty because of the lack of experimental data in the total and reaction cross sections. The decided OMP parameters produced the cross sections properly in the fast energy region. In the pre-equilibrium energy region, the direct and semi-direct capture model shows an improved fast neutron capture.

The calculated capture cross sections of Pd-107 and I-129 were in very good agreement with the reference measured data. The capture in ENDF/B-VI represented a somewhat difference from the calculation. The (n, p) and (n, 2n) cross section data were missed in ENDF/B-VI. Therefore, the current evaluated results will enhance the ENDF/B-VI. The elastic scattering cross section was created by the sum rule.

The evaluated results for the fast energy region were successfully merged with the resonance in an unresolved energy region. After a merging, the file experiences a physics checking using the CHECKR, FIZCON and PSYCHE codes. NJOY[5] code was run to check the file processing for real applications in many areas.

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