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Assessing the Impact on Criticality Calculations of LANL's New Cl Nuclear Data Evaluation

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1. Introduction

Recent studies on Molten Salt Reactor (MSR) development in Korea have examined chlorine (Cl) as a potential constituent of molten salts. It has been recognized that improvements in the nuclear reaction cross sections of Cl are necessary in the fast neutron energy range. Los Alamos National Laboratory (LANL) and TerraPower have produced new Cl cross section data based on neutron-induced charged-particle reaction measurement experiments and submitted them as candidate data for inclusion in the forthcoming ENDF/B-IX evaluation file. In this study, criticality benchmark calculations were performed using Cl data of ENDF/B-VIII.0[1], ENDF/B-VII.0[2], and LANL-TP, and the impact of Cl data on criticality was assessed. All calculations were performed using the MCNP6.2 code[3].

2. Cl Nuclear Reaction Cross Sections

In nature, Cl exists as two isotopes, Cl-35 and Cl-37, with abundances of 75.77% and 24.23%, respectively. Reviewing the evaluation history of Cl data since ENDF/B-VII.0, the Cl data in ENDF/B-VII.0 were produced by combining a file evaluated at LANL in 2000 with a resonance parameter evaluation performed at Oak Ridge National Laboratory (ORNL) in 2003. In 2007, ORNL revised the resonance parameter evaluation, which was subsequently incorporated into ENDF/B-VII.1[4]. The Cl evaluation in ENDF/B-VIII.0 incorporated an update to the prompt gamma-ray spectrum for thermal radiative capture (MF12 MT102) made by Lawrence Livermore National Laboratory (LLNL) and Lawrence Berkeley National Laboratory (LBNL) in 2015, as well as an update to the capture cross section above 1.2 MeV performed by LANL in 2016. The Cl data in ENDF/B-VIII.1[5] include the energy-angular distributions related to the emitted charged particles, updated by Korea Atomic Energy Research Institute (KAERI) and LANL in 2023.

Recently, under request from TerraPower, LANL conducted neutron-induced charged-particle reaction measurements using the LANSCE facility and newly obtained (n,p) and (n,α) reaction data for Cl. Based on these results, new Cl cross sections were evaluated and have been submitted for inclusion in the forthcoming ENDF/B-IX. Figures 1 ~ 4 compare the (n,p) and (n,α) cross sections of Cl-35 and Cl-37 from ENDF/B-VIII.0, ENDF/B-VII.0, and LANL-TP. The most significant difference among the evaluation files is the Cl-35 (n,p) cross section observed in the energy region above about 100 keV as shown in Fig. 1. The Cl-35 (n,p) cross section of LANL-TP appears as if it has returned to that of ENDF/B-VII.0. For the other reaction cross sections, ENDF/B-VIII.0 and ENDF/B-VII.0 are very similar, while LANL-TP shows slight differences.

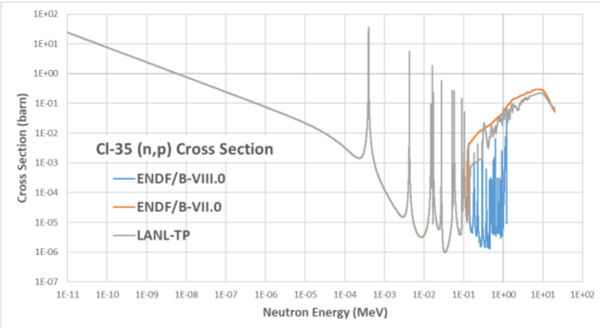

Fig. 1. Comparison of (n,p) reaction cross sections for Cl-35.

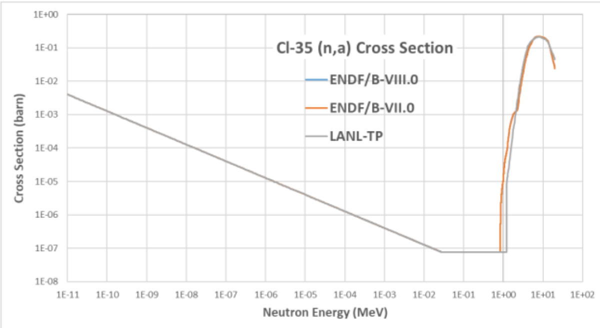

Fig. 2. Comparison of (n,α) reaction cross sections for Cl-35.

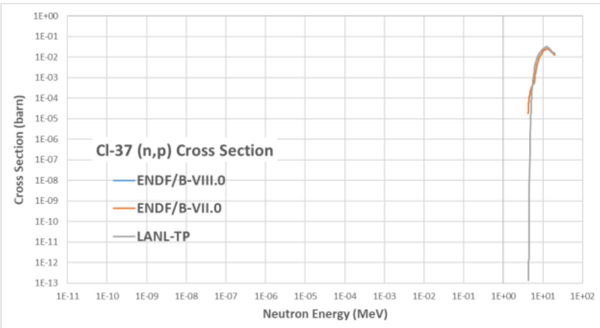

Fig. 3. Comparison of (n,p) reaction cross sections for Cl-37.

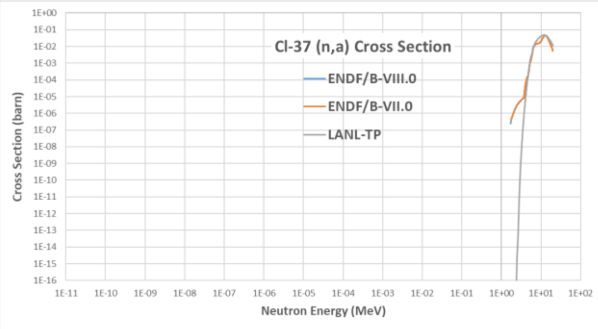

Fig. 4. Comparison of (n,α) reaction cross sections for Cl-37.

3. Criticality Benchmark Calculations

To examine the impact of Cl nuclear data on criticality calculations, 70 criticality benchmark problems containing Cl were selected using the Database for ICSBEP (DICE) tool of the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook[6]. These include 8 fast spectrum cases, 1 mixed spectrum case, and 61 thermal spectrum cases. Table I shows the ICSBEP problem IDs, the corresponding cases, and the types of Cl included.

Table I: Overview of ICSBEP Criticality Benchmark Problems

Problem ID	Case (# of Prob.)	Type of Chlorine
HEU-MET-FAST-056	001 (1)	Vermiculite
SUB-HEU-MET-FAST-001	001 (1)	Kel-F coating material, Sodium carbonate
IEU-MET-FAST-010	001 (1)	Core, Reflector
MIX-COMP-FAST-003	001, 002 (2)	Impurities
MIX-COMP-FAST-004	001 (1)	Impurities
MIX-COMP-FAST-005	001 (1)	Impurities
MIX-COMP-FAST-006	001 (1)	Impurities
SUB-HEU-MET-MIXED-001	001 (1)	Kel-F coating material
PU-SOL-THERM-009	001~003 (3)	Pu-solution(impurities)
PU-SOL-THERM-012	002~023 (22)	Lucoflex
HEU-SOL-THERM-003	001~019 (19)	Plexiglas
HEU-SOL-THERM-008	001~014 (14)	Plexiglas, Tailpipe
U233-SOL-THERM-003	041, 045, 055 (3)	Unichrome(PVC)

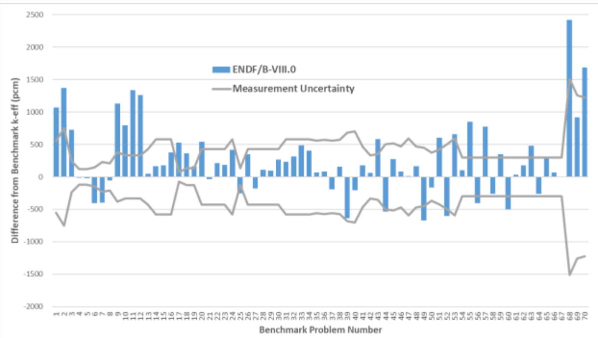

Fig. 5. Differences in k-eff between reference calculation using ENDF/B-VIII.0 and benchmark values.

Figure 5 shows the differences in k-eff between the reference calculation using ENDF/B-VIII.0 nuclear data and the benchmark k-eff values. For certain fast (hmf056-001, shmf001-001, imf010-001), mixed (shmm001-001), Pu thermal (pst009-001~003, pst012-006), HEU thermal (hst008-002, 004), and U233 thermal (ust003-041, 055) benchmark problems, the calculation results were found to greatly exceed the benchmark uncertainty.

Figure 6 shows the impact of the Cl data from ENDF/B-VII.0 and LANL-TP on criticality, in comparison with the reference calculation using ENDF/B-VIII.0. The Cl data of ENDF/B-VII.0 show an impact of about 99 pcm or more for pst012-016, hst003-005, and hst008-002. The Cl data of LANL-TP show a maximum impact of about 99 pcm in hst008-002, and about 73 pcm or more in hst003-006, 008, 013, and 017.

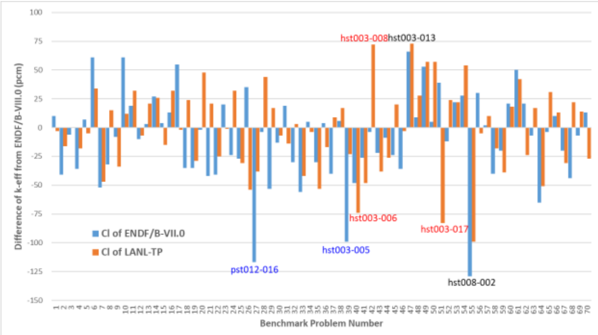

Fig. 6. Impacts of Cl data from other nuclear data files on k-eff relative to the reference calculation with ENDF/B-VIII.0.

Figure 7 shows the cumulative reduced chi-square values from the reference calculation results using ENDF/B-VIII.0 and from the calculation results with each Cl data. This value reflects not only the differences between the calculated and benchmark values, but also the magnitudes of the benchmark and calculation uncertainties. Gradual increases in slope correspond to cases with high calculation accuracy, yielding small chi-square contributions, whereas steep rises indicate cases with low calculation accuracy, typically when uncertainties are very small or when the differences from benchmark results are large.

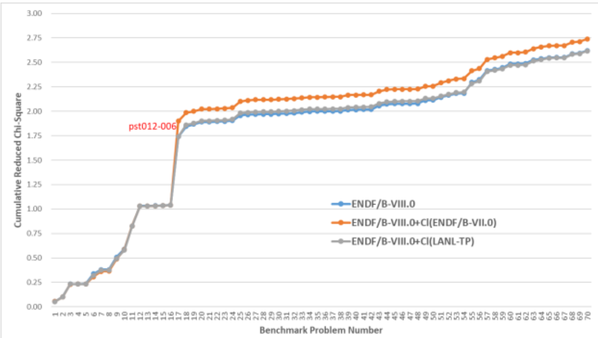

Fig. 7. Comparison of cumulative reduced chi-square values for different Cl nuclear data.

A typical example is the pst012-006 problem, which shows the most abrupt change in chi-square. In particular, for this case, the result using ENDF/B-VII.0 Cl data exhibits a relatively large deviation compared with the other calculations. In contrast, the result using the LANL-TP Cl data shows a trend very similar to the reference calculation. In terms of chi-square values, overall, the Cl data of ENDF/B-VIII.0 and LANL-TP show somewhat improved criticality calculation performance compared to that of ENDF/B-VII.0.

4. Summary

Criticality benchmark calculations were performed using the LANL-TP Cl data evaluated with recently measured neutron-induced charged-particle reaction experimental data from LANL, and the results were compared with those obtained using the Cl data from ENDF/B-VIII.0 and VII.0. A total of 70 benchmark problems were selected from the ICSBEP, among which the impact of the ENDF/B-VII.0 Cl data was the largest for the hst008-002 problem, at about 129 pcm. Compared with ENDF/B-VIII.0, the criticality impact was found to be more significant due to differences with the ENDF/B-VII.0 Cl data rather than changes in the LANL-TP Cl cross sections. It is considered necessary, in the future, to select appropriate benchmark problems in which the neutron spectrum is dominant in the energy range covered by LANL's measurements, in order to further assess the impact of the Cl data.

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