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Thought Experiment to Examine Benchmark Performance for Fusion Nuclear Data

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Abstract. There are many benchmark experiments carried out so far with DT neutrons especially aiming at fusion reactor development. These integral experiments seemed vaguely to validate the nuclear data below 14 MeV. However, no precise studies exist now. The author's group thus started to examine how well benchmark experiments with DT neutrons can play a benchmarking role for energies below 14 MeV. Recently, as a next phase, to generalize the above discussion, the energy range was expanded to the entire region. In this study, thought experiments with finer energy bins have thus been conducted to discuss how to generally estimate performance of benchmark experiments. As a result of thought experiments with a point detector, the sensitivity for a discrepancy appearing in the benchmark analysis is “equally” due not only to contribution directly conveyed to the deterctor, but also due to indirect contribution of neutrons (named (A)) making neutrons conveying the contribution, indirect controbution of neutrons (B) making the neutrons (A) and so on. From this concept, it would become clear from a sensitivity analysis in advance how well and which energy nuclear data could be benchmarked with a benchmark experiment.

1 Introduction

There are a lot of nuclear data measurements, named differential experiments, carried out so far with DT neutron sources. Also there exist many benchmark experiments, i.e., integral experiments, to verify the nuclear data validity. They are of course aiming at fusion reactor development finally. Differential experiments can check the accuracy of evaluated nuclear data at 14 MeV directly. Integral experiments are vaguely expected to validate the nuclear data also below 14 MeV as well as at 14 MeV. However, no precise studies concerning this matter were performed systematically so far. On the other hand, as for numerical calculations with transport codes, it is quite common to analyze benchmark experiments using Monte Carlo codes. It would become very useful if benchmark performance for nuclear data could directly be analyzed beforehand from the Monte Carlo calculations. In the author’s group, various fusion neutronics experiments have been carried out so far with a 14 MeV neutron source, OKAVIAN. We thus started to examine how well integral benchmark experiments with DT neutrons can play a benchmarking role for energies below 14 MeV using a general purpose Monte Carlo code MCNP.[1)]

We calculated an energy spectrum of neutrons making neutrons or gamma-rays detected by a detector in a leakage neutron or gamma-ray spectrum measurement. This spectrum was named “neutron spectrum before last collision”, φ_{last}, in this study. Calculation of φ_{last} was done with a point detector as in the following procedure. For each detected contribution, there exists a neutron or gamma-ray, named (A), conveying the contribution to the detector. The information, i.e., the contribution and energy of (A) is summed up to make a measured spectrum in the calculation. Now, we think of another neutron (B), making the neutron or gamma-ray, (A), conveying the contribution. The spectrum of φ_{last} can be evaluated by contribution conveyed by particle (A) with the energy of particle (B) instead of (A).

As a result of the series study[2,3)], especially for DT neutron benchmark experiments, it was found that for secondary gamma-ray spectrum measurements nuclear data at around 14 MeV were dominantly benchmarked. In return, for neutron spectrum measurements those below 14 MeV were also benchmarked fairly well in addition to 14 MeV, because neutrons could rapidly be moderated in a sample material. In conclusion, to make benchmark experiments efficient, a spectrum shifter made with beryllium should be used to make the incident neutron spectrum softer especially for gamma-ray spectrum measurements. For neutron spectrum measurements, it was pointed out that reduction of experimental time could be expected.

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In benchmark analyses carried out so far[2,3], we set only one energy boundary at 10 MeV to examine φ_{last}, meaning the number of energy groups is just two (14 MeV and other than 14 MeV), because the incident particle is a mono-energetic 14 MeV neutron and we wanted to know simply if the measured neutron spectrum below 14 MeV could validate the nuclear data not only for 14 MeV but also below 14 MeV. This concept worked well for performance analysis of the benchmark with DT neutrons. But in general cases it seemed to be insufficient to employ one boundary. The key point is how we should make a discussion in the general cases in the same manner as the case of two energy groups. As shown in **Fig. 1** which is the case of a leakage neutron spectrum by DT neutrons, it is found that neutrons (B) are already staying in a bin close to the energy bin of neutrons (A). In this sample size (about several tens cm thick), it can be found that the neutron spectrum mostly reaches its equilibrium one. For gamm-ray spectrum case in **Fig. 2**, in contrary, gamma-rays produced by 14 MeV neutrons are found to be dominant. It means especially for neutrons that finer energy meshes are essential and indispensable in general cases. Consequently, two problems were pointed out to discuss the benchmark performance in Ref. 3).

Here, one of the two is introduced, because it is directly related to the present objectives. In our previous studies the problem did not explicitly appear, because the energy boundary is only at 10 MeV, meaning that only 14 MeV neutrons and neutrons below 14 MeV exist. However, if using finer energy bins, there must exist various energetic neutrons, i.e., neutrons (A) conveying contribution to a certain energy mesh of the spectrum, neutrons (B) making neutrons (A), neutrons (C) making neutrons (B) and so on. The key issue is that one has to think of not only neutrons (A) but also other neutrons created during the whole particle history from the source.

In the present study, we carry out a thought experiment to precisely examine which neutron, i.e., nuclear data for the neutron energy, created during a transport history is benchmarked by the measured detector contribution. The change appearing in the measured spectrum is examined, if the cross section value were artificially changed to be a little over- or underestimated. From the result, the benchmark performance sensitivity due to discrepancy between measurement and calculation is discussed. Investigating the whole thought experiment, we discuss how well neutrons created during the transport are benchmarked. And finally we examine that we reach the conclusion that there would be no need to calculate adjoint function for benchmark performance (sensitivity) analysis.

2 Thought Experiment

As a thought experiment, we think of a DT neutron incidence to a sample as shown in **Fig. 3**. The sample is so thin that it can be assumed that scattering occurs just twice at maximum. Also, assuming that emitted secondary neutrons via first and second scattering can be measured separately. It means that the spectrum from the first scattering corresponds to double differential cross section (DDX) and the second one is a distortion term by scattering. The mixture of the two is a neutron spectrum to be measured.

In the separate measuremtn, we think of how effectively each spectrum plays a benchmarking role. Naturally, the neutron spectrum made directly from the first scattering plays a benchmarking role for the incident 14 MeV neutrons (n_0). In this case the contribution is conveyed by neutrons (n_1) to the detector. The second spectrum is made up of contributions created by neutrons (n_1) emitted via nuclear reactions of the incident neutrons (n_0). The contributions are delivered by neutrons (n_2). Therefore, the spectrum can play a benchmarking role for n_1. The point is 'whether the second one could have a benchmarking role also against the incident neutrons (n_0)'. Seemingly, it is quite likely, because neutrons (n_1) producing the second spectrum are originally created by neutrons (n_0). Now, the problem is, if so, 'whether the benchmark performance degree for both of n_0 and n_1 is the same'.

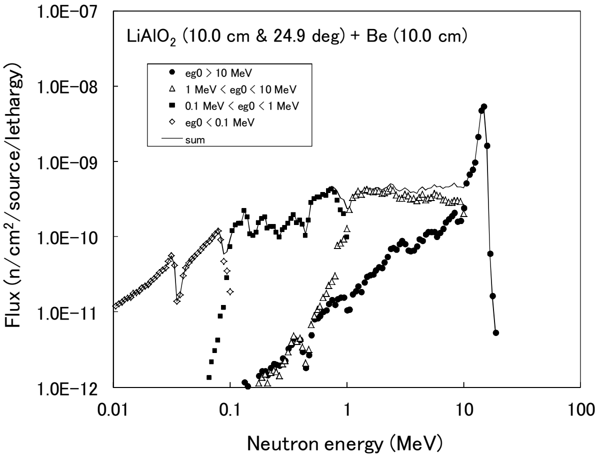

Fig. 1. Calculated leakage neutron spectrum for Li_2TiO_3 by DT neutrons. 'eg0' is the energy of neutron spectrum before last collision, φ_{last}, and 'sum' is the calculated neutron spectrum. ●,△,■ and ◇ indicate to partial spectra made by each φ_{last}.

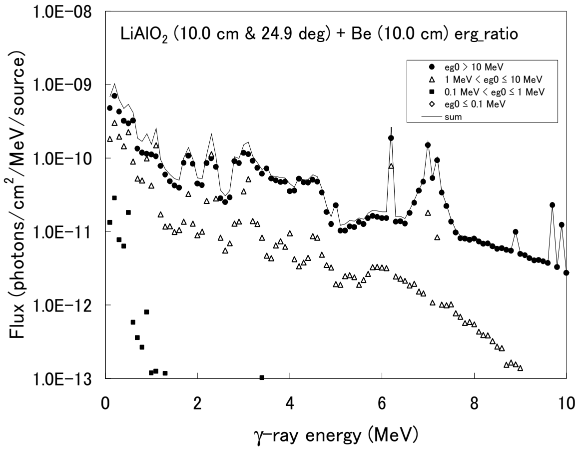

Fig. 2. Calculated leakage gamma-ray spectrum for Li_2TiO_3 by DT neutrons. Other condition is the same as Fig. 1.

Table 1 Error sensitivity analysis result in a simple benchmark model.

	Cross section assumption		Comparison of experiment and calculation		
	14 MeV	Below 14 MeV	n_1 spectrum	n_2 spectrum	Total
(1)	–10 %*1	Correct	–10 %*2	–10 %	–10%
(2)	Correct	–10 %	Correct	–10 %	Underestimated a little*3
(3)	–5 %	–5 %	–5 %	–5 ～ –10%	–5 ～ –10%*4

*1 Cross section is assumed to be underestimated. *2 Underestimation of calculation
*3 Because n_1 spectrum is dominant. *4 The value is expected to be close to -5%.

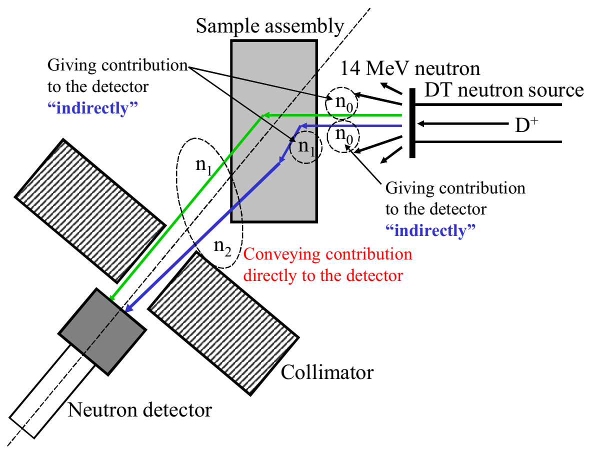

Fig. 3 Schematic arrangement of neutron benchmark experiment for the thought experiment.

2.1 Simple benchmark sensitivity

Now thinking of a similar benchmark experiment to Fig. 2 with a relatively thin slab sample, the benchmark sensitivity is examined with a simple condition as follows: Assuming cross sections except 14 MeV are correct, and that of 14 MeV is underestimated by 10 % (By this, the produced DDX by 14 MeV neutron shows a little smaller spectrum by 10 %.) In this case, if comparing the measured spectrum with the calculation, the calculated n_1 spectrum shows 10 % smaller in the whole energy region. This means that the number of neutrons making the second spectrum is decreased by 10 %. Thus, the spectrum of n_2 neutrons produced by n_1 shows 10 % smaller also. As a total of n_1 and n_2, the estimated measured spectrum shows 10 % smaller. The result is summarized in **Table 1**. The above result indicates that both spectra due to the first and second scatterings play equally the benchmarking role at the energy of 14 MeV.

Inversely, assuming the cross section of 14 MeV is correct and others below 14 MeV are smaller by 10 %, a similar simple thought experiment is done as follows: The n_1 spectrum calculated is clearly correct (showing the same as the measurement). As for the n_2 spectrum, the absolute value becomes smaller by 10 % because of 10% smaller cross sections for neutrons n_1, although the intensity of neutrons n_1 (produced as a result of the first scattering by n_0) making the n_2 spectrum is correct. The summed-up spectrum to be measured shows a smaller value by less than 10 %, probably the absolute value is smaller, because in reality the spectrum of n_1 is dominant.

Then, in case of the cross section being 5 % smaller in both energy ranges, meaning 5 % smaller in the whole energy range, the n_1 spectrum shows 5 % smaller. Because the spectrum of neutrons making the n_2 spectrum is also 5 % smaller, the n_2 spectrum has to be smaller by 5 %. The total result shows a decrease of between 5 and 10 %, probably close to -5%.

In summary, when the calculated spectrum shows a 10 % smaller value in energies below the elastic peak of 14 MeV compared to an experiment, the benchmark activity is to find out the reason why the discrepancy happens. From the above sensitivity analysis, it would be the most likely that the cross section of 14 MeV would be wrong (smaller), then second-likely that both would be underestimated, and the probability is the smallest that the cross sections only below 14 MeV are incorrect.

The important conclusion is that this kind of evaluation is of course not possible if only neutron spectrum before last collision is taken into consideration.

2.2 Precise benchmark sensitivity

Based on the results obtained above, a more precise benchmark sensitivity is next examined with a practical model, that is, a leakage spectrum measurement with a slab assembly by 14 MeV neutron incidence. Here, we focus on an energy bin of 5 to 6 MeV, for example, in the measured spectrum. Similar to the previous section, the number of scatterings is assumed to be up to twice. In this case, some measured neutrons may be produced by 14 MeV neutron's nuclear reactions, and some others may be via nuclear reactions by neutrons below 14 MeV, which are created by the 14 MeV neutron's nuclear reactions. The former measured neutrons are named n_1, and the latter is n_2, in the same manner as the previous section. Now, we employ the following assumption additionally that the ratio of the detector contribution in the energy bin conveyed by n_1 is $1–a$ ($0 < a < 1$), and that by n_2 is a as shown in **Fig. 4**. So, if the C/E is 0.9 and the error contribution is simply proportional to contribution of the whole spectrum, it could be expected

Table 2 Error sensitivity analysis result in a precise benchmark model.

Measured	n_1 spectrum	n_2 spectrum	Error sensitivity to the energy bin	Total	Ratio	Expectation
10 % underestimated nuclear data at 14 MeV and correct for others to examine n_0 sensitivity						
n_1	–10 %	–	–10(1–a) %	–10 %*2	1	1– a
n_2	–10 %*1	–10 %	–10a %			
Correct nuclear data for 14 MeV and 10 % underestimated for others to examine n_1 sensitivity						
n_1	0	–	0	–10a %*3	a	a
n_2	0*1	–10 %	–10a %			

*1 As a source to make n_2. *2 n_0 sensitivity *3 n_1 sensitivity

that the origin of the error, 10%, could be divided into –10(1–a) % for 14 MeV neutrons and –10a % for n_1, because n_1 is produced by a 14 MeV neutron and n_2 is produced by n_1. However, as detailed in the following, it will be made clear that this is not the case.

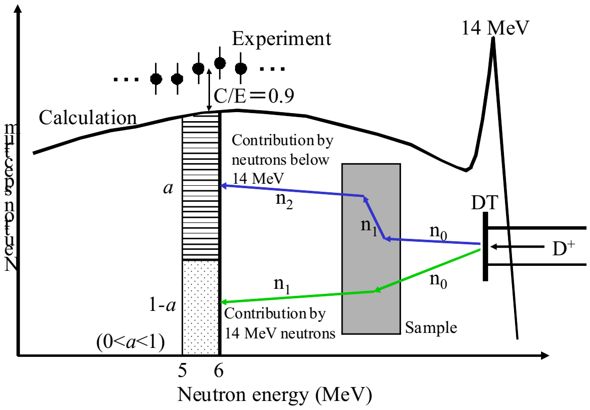

Fig. 4 Detector contribution ratio a in neutron spectrum.

In the condition above, from the result in Sec. 2.1, it can be expected that the probability is larger that the cross section of 14 MeV is incorrect. In other words, the crucial point is that n_1 is the source term to make n_2. Again we think of the condition, C/E=0.9.

At first it is assumed that the cross section at 14 MeV is underestimated by 10 % and others are correct. In this case, as shown in **Table 2**, the calculated n_1 spectrum shows an underestimated result by –10 %, and the error sensitivity of bin 5~6 MeV due to n_1 is estimated to be –10(1–a) %. Though cross sections of scattering induced by n_1 are correct, the spectrum of n_1 as a source term for the following nuclear reaction is smaller by –10 %. The calculated spectrum of n_2 thus becomes –10 %, because other cross sections than 14 MeV are assumed to be correct. Consequently, The error sensitivity of bin 5~6 MeV due to n_2 is –10a %. As a result, the total sensitivity of the bin is calculated by summing up n_1 and n_2 error sensitivities, i.e., –10 %.

Second, it is assumed that the cross section at 14 MeV is correct and others are underestimated by 10 %. In this case, the calculated spectrum of n_1 is correct, and the error sensitivity of bin 5~6 MeV due to n_1 is estimated to be zero. The spectrum of n_1 as a source term for the following nuclear reaction is also correct. However, the spectrum of n_2 possesses –10 % error, because other cross sections than 14MeV are assumed to be underestimated by 10%. The error sensitivity of bin 5~6 MeV due to n_2 is thus –10a % and the total sensitivity of the bin is thus –10a %.

As a sensitivity ratio, 14 MeV : Others = 1 : a, meaning the probability is higher that the cross section at 14 MeV is not correct, as expected also in Sec. 2.1. However, as described earlier it was expected the ratio is 1–a : a. Both conclusions do not agree with each other. In the next section, the reason why the disagreement appears will be made clear.

2.3 Benchmark sensitivity contribution of each scattering neutron

In the beginning of Sec. 2.2, out of the contribution in the bin 5~6 MeV, it was seemingly expected that the ratio of 1–a came from n_1 and ratio, a, from n_2. However, this was available in case that we focused just on neutrons before last collision. In the conclusion of Sec. 2.2, considering another nuclear reaction forming spectrum n_2, the error sensitivity became

$$14 \text{ MeV} : \text{Others} = 1 : a \qquad (1).$$

In fact, this sensitivity is deeply related to the place where detector contribution comes from. Practically, n_2 surely conveys contribution a in the energy bin 5～6 as shown in Fig. 4. However, n_2 is created by n_1 via nuclear reaction. It means that it can be said that n_1 would convey the contribution indirectly to the detector. More precisely, it can be concluded from a physical consideration with 'importance' proposed by Lewins[4)] with the result in Table 2 that "Error sensitivity for a certain neutron is proportional to the total detector contribution neutrons give directly and indirectly." Concretely, the detector contribution 14 MeV neutrons, n_0, give includes partly contribution, 1–a, through neutron n_1 as shown in **Table 3**. This is a direct contribution made by a 14 MeV neutron. And there is another contribution of n_1, a, conveyed by n_2. n_2 is made by n_1's nuclear reaction. This is also a direct contribution of n_1 conveyed by n_2. Since n_1 is created by n_0, it can be thought that n_0 has an indirect contribution a. This is the same concept as 'importance' proposed by Lewins. As a result, n_0 has direct contribution, $1-a$, and indirect contribution, a, leading to the conclusion that n_0 has the total contribution,

$$(1 - a) + a = 1 \quad (2).$$

On the other hand, the contribution of other neutrons, n_1, is just a, directly made by themselves. Consequently, the detector contribution ratio can be estimated to be

$$14 \text{ MeV} : \text{Others} = 1 : a \quad (3),$$

as summarized in Table 3. This result is surprisingly the same as the error sensitivity ratio discussed in Sec. 2.2 and shown in Table 2.

Now, the problem is why the above expectation holds. The error sensitivity of 14 MeV neutrons in the case of assuming cross sections except 14 MeV are correct and that of 14 MeV is underestimated by 10 %, described in the previous section, shows

$$-10(1-a)\ \% + (-10a\ \%) = -10\ \% \quad (4).$$

It seems that a sensitivity of neutrons other than 14 MeV, that is, $-10a$ % is added. This is just caused by the fact that 14 MeV neutrons produce n_1. More practically, underestimation of cross section at 14MeV propagates in the lower energy neutrons, n_1, created by n_0. This is the indirect contribution. If removing an initially given error of –10 %, the total ratio unity in Table 2 is exactly the same as the contribution summation calculation just above. On the other hand, the error sensitivity of other neutrons n_1 in Sec. 2.2 is $-10a$ %. This just means if removing –10 %, the term a is left, which is similarly the same as the contribution in Table 3.

Table 3 Direct/indirect contribution ratio to the detector.

Contribution	Direct	Indirect	Total
14 MeV (n_0)	$1-a$	a	1
Others (n_1)	a	–	a

The discussion carried out so far concludes as follows: In case of benchmarking the nuclear data with a measured neutron or gamma-ray spectrum, if any discrepancy appears, one wants to know which energy neutrons are concerned for this discrepancy. Or before benchmark experiments, one wants to know in which energetic neutrons the expeiments benchmark. According to the present thought experiments, the benchmark sensitivity for the experiment is “equally” due not only to neutrons (named (A)) making neutrons conveying contribution directly to the deterctor, but also due to neutrons (B) making neutrons (A). In this case, it can be recognized that neutrons (B) convey the same contribution indirectly through (A), which is called indirect contribution. Similarly neutrons (C) making (B) have the same indirect contribution as (B) and so on, i.e., all the ancestor neutrons have the same contribution (error sensitivity). This gives us an very important hint for the benchmark error sensitivity as in the following section:

2.4 Benchmark sensitivity with Lewins importance in forward Monte Carlo calculations

As Lewins proposed[4)], in particle transport calculations, importance is regarded as contribution each particle has. The Lewins’ contribution is defined as all the contribution which will be made by all the progenies of the particle in the whole transport calculation. According to the present thought experiments, it was found that the contribution governing the error sensitivity in Table 3 was exactly the same as the Lewins’s contribution (importance). It means that benchmark error sensitivity could be evaluated by importance which can be estimated by forward Monte Carlo calculations. It also means error sensitivity could be predicted in forward Monte Carlo calculations, i.e., without adjoint function.

As a next phase, a more theoretical approach to form the mathematical expression with the present thought experiment and Lewins’ style importance. And practical Monte Carlo calculations are planned to carry out to confirm the validity.

3. Conclusion

Thought experiments have been conducted to discuss how to estimate performance of benchmark experiments for neutron nuclear data for fusion reactor design. We carried out simple and precise thought experiments to examine which energy neutron is deeply concerned to the discrepancy, in case that there appears discrepancy between an experiment and its analysis with a transport code. As a result of the thought experiments, the benchmark sensitivity is “equally” due not only to neutrons (named (A)) making neutrons conveying contribution directly to the deterctor, but also due to neutrons (B) making neutrons (A). The neutrons (B) convey the same contribution indirectly through (A), which is called indirect contribution. Similarly all the ancestor neutrons have the same contribution (error sensitivity), which is an indirect contribution.

The above result leads the following conclusion: Because the Lewins’s contribution (importance) is exactly the same as contribution governing the error sensitivity, benchmark error sensitivity could be evaluated by importance which can be estimated by forward Monte Carlo calculations. It also means error sensitivity could be predicted in forward Monte Carlo calculations, i.e., without adjoint function. With this procedure, it would become possible that from a sensitivity analysis in advance we could know how well and which energy nuclear data could be benchmarked with a benchmark experiment.

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