

Remarks on LLNL pulsed sphere work (part II)

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UPM is collaborating with LANL, IAEA/NDS and JSI ...

1. Collection of TOF Shielding Benchmarks for Nuclear Data validation

- **LANL** is working to understand which nuclear-data observables can be validated with pulsed spheres...
 - See presentation in WPEC/SG47 May 2020, “Using LLNL Pulsed Spheres for Nuclear Data Validation”, D. Neudecker.
 - **75 LLNL pulsed-sphere neutron-leakage spectra for 20 different materials.**

2. Sensitivity Analysis... in LLNL pulsed spheres

- ... **LA-UR-20-26735 (2020-08-31)**

“Sensitivity Analysis of Neutron-leakage Spectra for a Small Suite of LLNL Pulsed Spheres to $MF = \{1, 3, 5\}$ Nuclear Data”. O. Cabellos, D. Neudecker

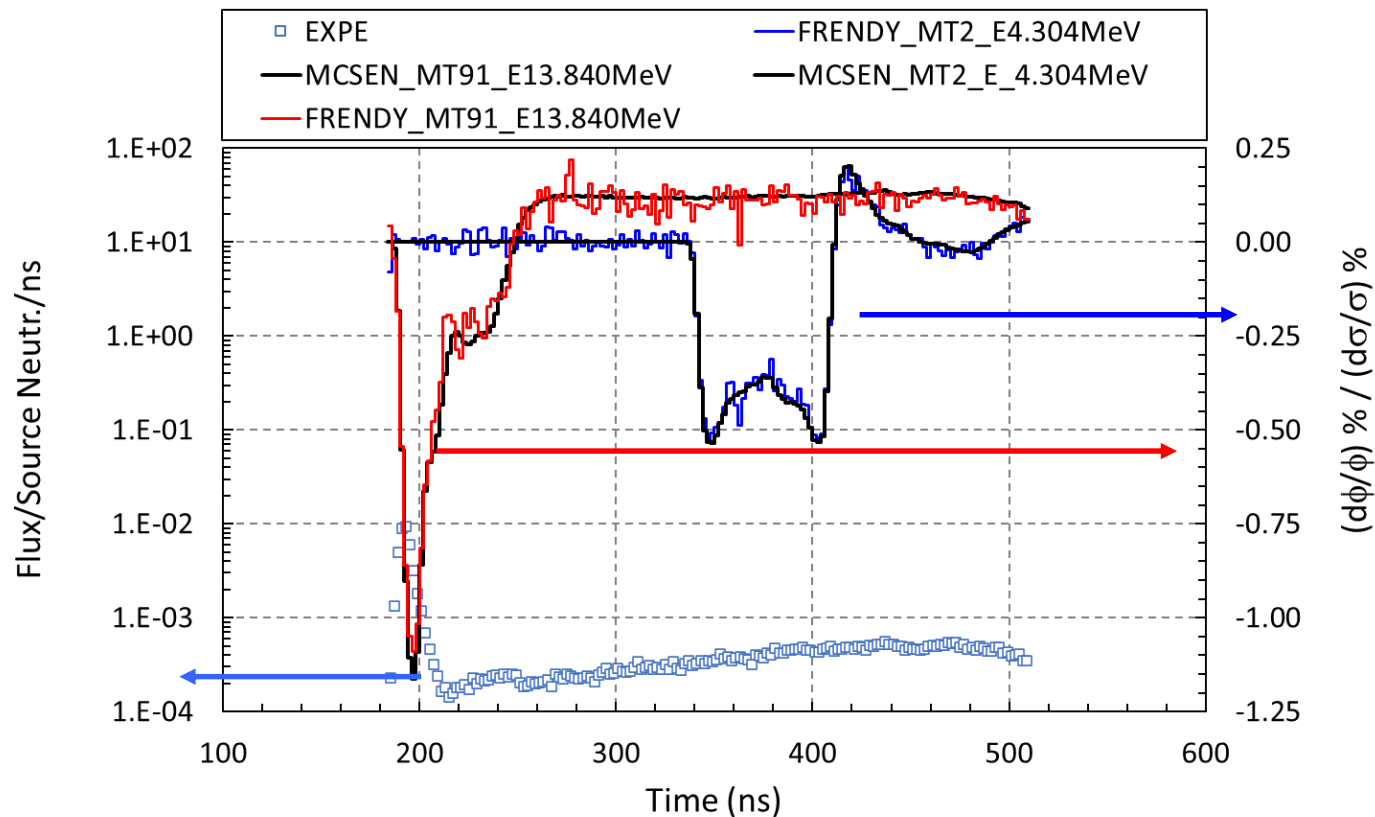
- ... **paper to be published in Annals of Nuclear Energy**

“Which nuclear data can be validated with LLNL pulsed-sphere experiments ?” D. Neudecker, O. Cabellos, A.R. Clark, W. Haeck, M. C. White, R. Capote, A. Trkov, M. Rising

- ❑ Methodology for providing sensitivity profiles
 - **MCSEN code**
 - **MCSEN5 -> MCNP5.1.30 (problems for new ND evaluations)**
 - R.L. Perel, J.J. Wagschal, Y. Yeivin, “Monte Carlo Calculation of Point-Detector Sensitivities to Material Parameters”, Nuclear Science and Engineering, 124 (1), 197–209 (1996)
 - MCSEN is able to operate on: cross-sections, nubar, CHI and MF4 and MF6
 - **SANDY and FRENDY codes using perturbation capabilities**
 - **SANDY** (<https://github.com/luca-fiorito-11/sandy>)
 - SANDY perturbs either ENDF or PENDF files
 - Process ENDF/PENDF files into ACE format with NJOY
 - SANDY is able to operate on: cross-sections, nubar, CHI and MF4 (soon on MF6)
 - **FRENDY** (https://rpg.jaea.go.jp/main/en/program_frendy/)
 - FRENDY directly perturbs ACE files
 - FRENDY is able to operate on: cross-sections, nubar and CHI

❑ Comparison of Sensitivity profiles: MCSEN versus FRENDY

LLNL Pulsed Sphere: fe4.8: Example of Sensitivity Profiles for ^{56}Fe





Which nuclear data can be validated with LLNL pulsed-sphere experiments?☆

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ANE Special Issue on "A tribute to Massimo Salvatores, a great scientist and a great man"

❑ Sensitivity profiles for LLNL pulsed spheres

- **“Sensitivity profiles of the spectra to nuclear data are calculated in order to understand in detail which isotopes, observables, and energy ranges of nuclear data contribute significantly to their simulation”**
- Few selected spheres containing different materials, the neutron-leakage spectra is sensitive to :
 - For spheres containing **light elements** (^{16}O , ^{12}C) is mostly sensitive to elastic- and inelastic-scattering cross sections on discrete levels and corresponding angular distributions
 - For spheres of **structural materials** (^{56}Fe) are sensitive to elastic-and inelastic-scattering cross sections, including scattering on discrete levels and the continuum, and double-differential cross sections.
 - For **actinide spheres** (^{239}Pu) are also strongly sensitive to the fission observables, in particular to the total-fission neutron spectrum.
- In regards of thickness:
 - **Thin spheres** (in which neutrons experience on average less than one scatter) are mostly sensitive to data near the elastic peak, in the energy range from 12–15 MeV
 - **Thicker spheres** can be sensitive to data at lower incident-neutron energies due to multiple-scattering effects

□ Sensitivity profiles for LLNL pulsed spheres

Table. List of all pulsed-sphere experiments for which sensitivity profiles are studied here is given. They are identified by their material, reference used for generating the input deck (Ref.), mean free path (mfp), detector, angle, year of reference, and light-path length, “*l*”.

Material	Ref.	Mfp	Detector	Angle	Year	<i>l</i> (cm)
Light water	[5]	1.9	NE213-A	117	1972	975.4
Heavy water	[5]	1.2	Pilot-B	39	1972	765.2
⁶ Li	[5]	1.6	NE213-B	26	1972	746.3
Polyethylene	[5]	3.5	Pilot-B	39	1972	765.2
Carbon	[5]	2.9	NE213-A	117	1972	975.2
¹⁶ O	[5]	0.7	Pilot-B	39	1972	754.0
Concrete	[5]	2.0	NE213-A	117	1972	975.4
Teflon	[5]	2.9	NE213-A	117	1972	975.4
Magnesium	[5]	0.7	NE213-A	117	1972	977.2
²⁷ Al	[5]	0.9	NE213-A	117	1972	977.2
Iron	[5]	4.8	NE213-A	117	1972	975.2
Lead	[5]	1.4	NE213-A	117	1972	975.2
²³⁵ U	[7]	0.7	NE213-B	26	1976	945.5
²³⁸ U	[7]	0.8	NE213-A	117	1976	977.2
Plutonium	[7]	0.7	NE213-A	117	1976	975.2

□ Sensitivity profiles for LLNL pulsed spheres

Table. The nuclear-data observables that were perturbed for each isotope studied here are given in the MF/ MT nomenclature.

Isotope/ Element	MF, MT numbers
¹ H	MF=3: MT=2, 102; MF=4: MT=2
² H	MF=3: MT=2, 16, 102; MF=4: MT=2
^{6,7} Li	MF=3: MT=2, 4; MF=4: MT=2 (^{6,7} Li), 51, 52 (⁷ Li)
C	MF=3: MT=2, 4, 51, 91, 102; MF=4: MT=2, 51, 52
¹⁶ O	MF=3: MT=2, 4, 51, 91, 102; MF=4: MT=2, 51, 52
¹⁹ F	MF=3: MT=2, 4, 16
²⁴⁻²⁶ Mg	MF=3: MT=2, 4, 91; MF=4: MT=2, 51, 52 (only ^{24, 25} Mg)
²⁷ Al	MF=3: MT=2, 4, 28, 51, 91, 102, 103, 107; MF=4: MT=2, 51, 52
²⁸ Si	MF=3: MT=2, 4, 91, 103, 107; MF=4: MT=2
⁴⁶ Ti	MF=3: MT=102
^{47,49,50} Ti	MF=3: MT=2
⁴⁸ Ti	MF=3: MT=2, 4, 91
^{54,56} Fe	MF=3: MT=2, 4, 16, 51, 91, 102, 107; MF=4: MT=2, 51,52; MF=6; MT=91
²⁰⁶⁻²⁰⁸ Pb	MF=3: MT=2, 4, 16, 91; MF=4: MT=2, 51, 52 (²⁰⁶ Pb only)
^{235,238} U	MF=1: MT=452; MF=3: MT=2, 4, 18, 51, 91, 102; MF=4: MT=2, 51, 52 (only ²³⁸ U); MF=5: MT=18
^{239,240} Pu	MF=1: MT=452; MF=3: MT=2, 4, 18, 51, 91, 102; MF=4: MT=2, 51, 52 (only ²³⁹ Pu); MF=5: MT=18; MF=6, MT=91

❑ Sensitivity profiles for LLNL pulsed spheres. An example: ^{16}O -0.7mfp

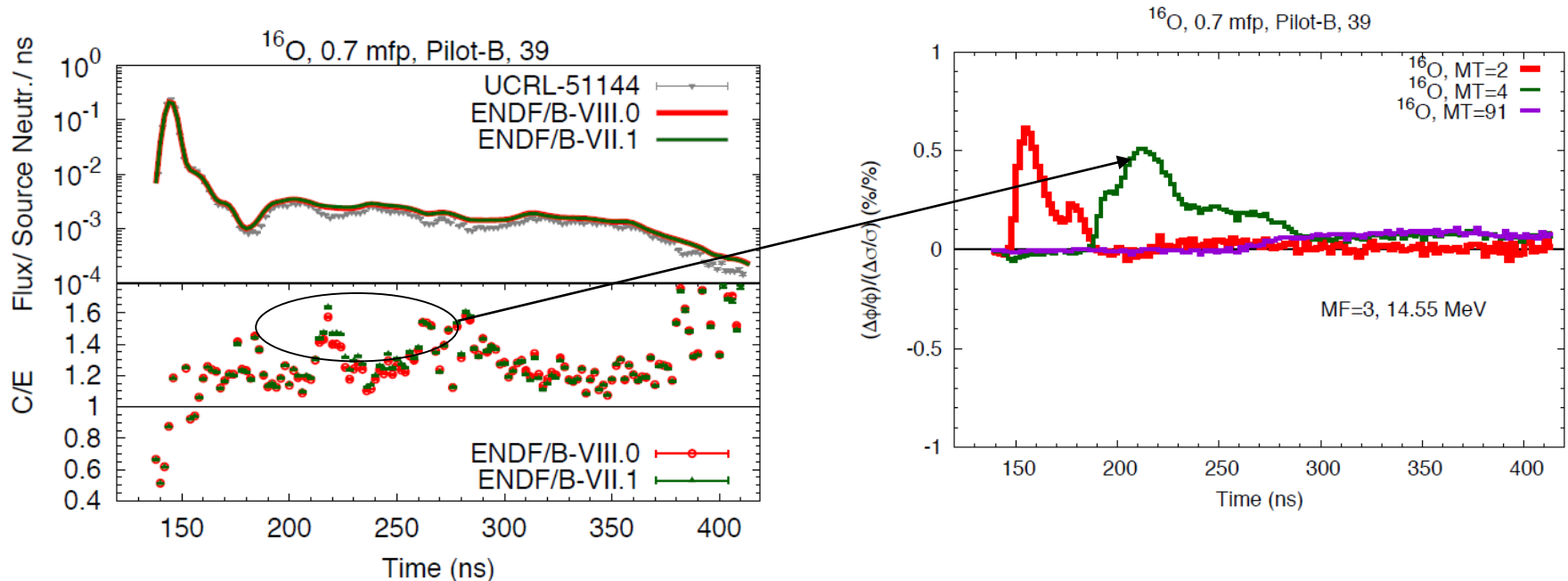


Figure. ^{16}O LLNL pulsed-sphere experimental data compared to MCNP simulations using ENDF/B-VII.1 and ENDF/B-VIII.0.

Figure. Sensitivities of ^{16}O pulsed-sphere neutron-leakage spectra to various cross sections for the same incident-neutron energy. The energy given in the label is the maximum energy of the bin-in this case, energies from 13.84-14.55 MeV.

- ❑ C/E values are overpredicted by as much as 60%
- ❑ Deficiencies shown from 200-300 ns could be possibly associated with deficiencies in the inelastic-scattering?

□ Sensitivity profiles for LLNL pulsed spheres . An example: ^{16}O -0.7mfp

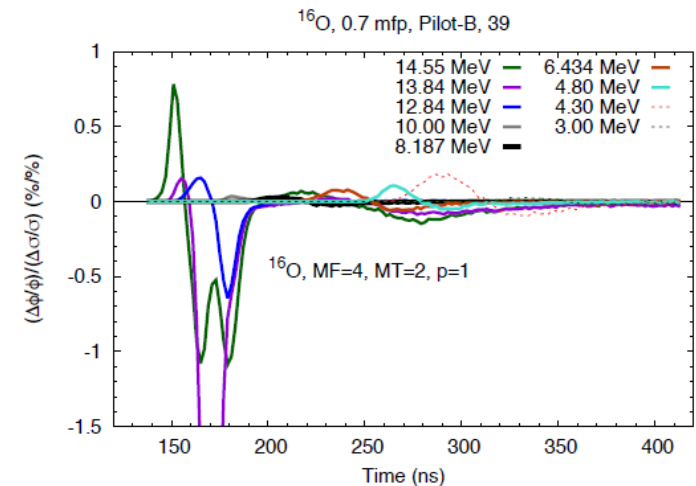
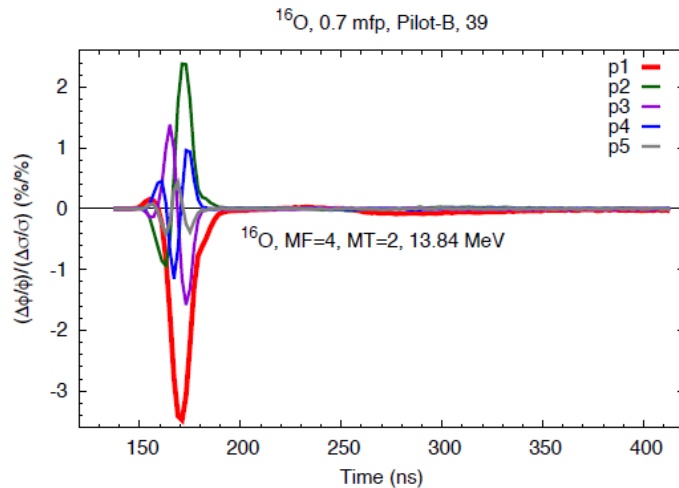
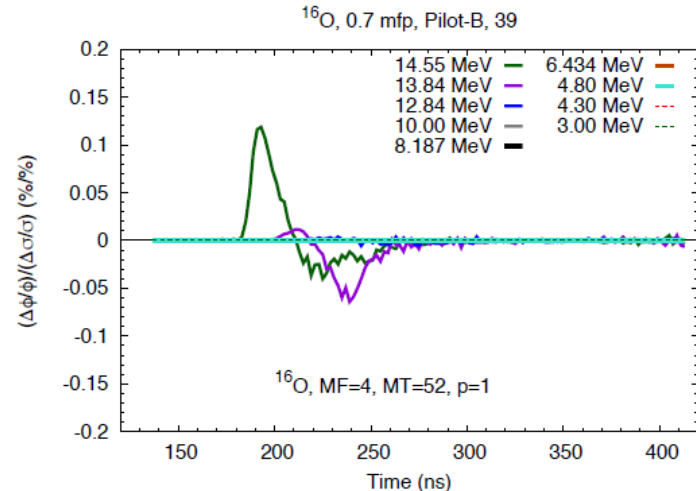


Figure. Sensitivities of ^{16}O pulsed-sphere neutron-leakage spectra to **Legendre coefficients** of elastic - and inelastic-scattering angular distributions with maximum absolute values of more than 0.05 %/ %.



- Large sensitivities for elastic - and inelastic - scattering cross sections in the 12-15 MeV range will be associated with elevated sensitivities to the corresponding angular distributions
- There is a significant sensitivity to $^{16}\text{O}(n,\text{el})$ **Legendre coefficients**

❑ Sensitivity profiles for LLNL pulsed spheres . An example:¹⁶O-0.7mfp

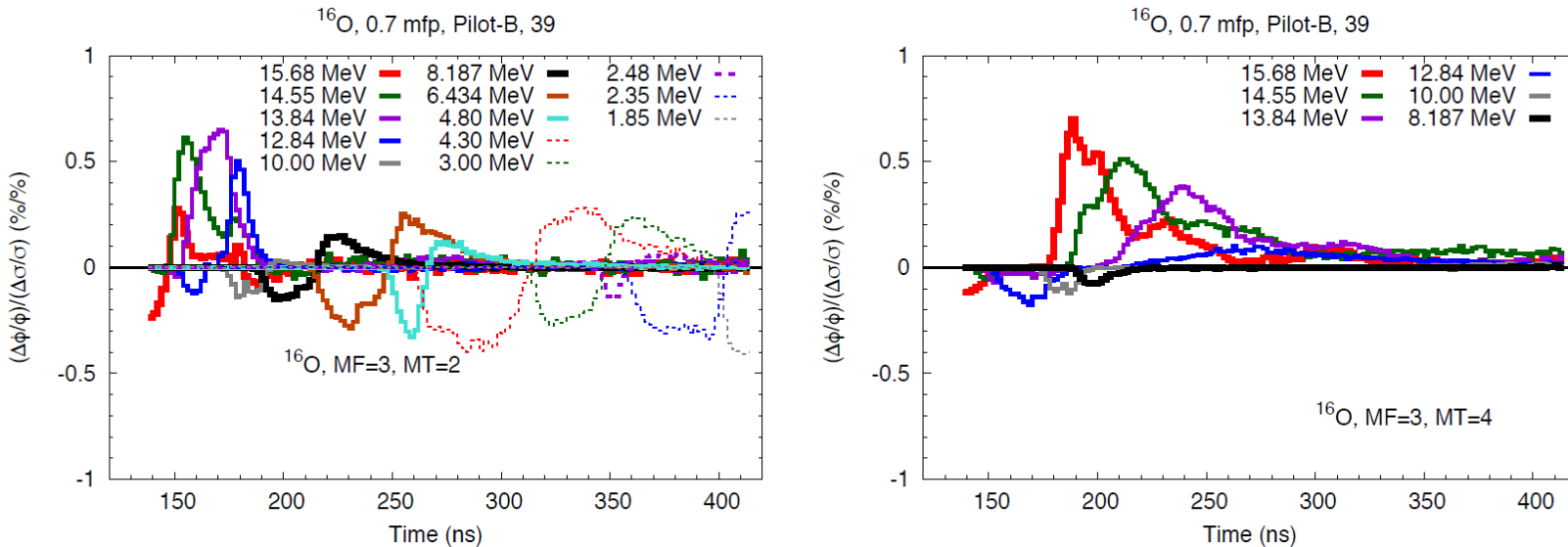


Figure. Sensitivities of ¹⁶O pulsed-sphere neutron-leakage spectra to elastic (MF=3, MT=2) and inelastic (MF=3, MT=4) cross sections.

- ❑ All sensitivities to XSs have in common is that they are **negative at low tof and positive at higher tof**
- ❑ For elastic scattering, the neutrons are deflected in angle to be measured at approx. 39°. This deflection leads to a longer flight-path than when measured at 0° to the deuteron beam resulting to be measured at later tof
- ❑ For inelastic scattering, the sensitivity is spread out to even larger tof given the loss of energy

❑ Sensitivity profiles for LLNL pulsed spheres . An example: ^{16}O -0.7mfp

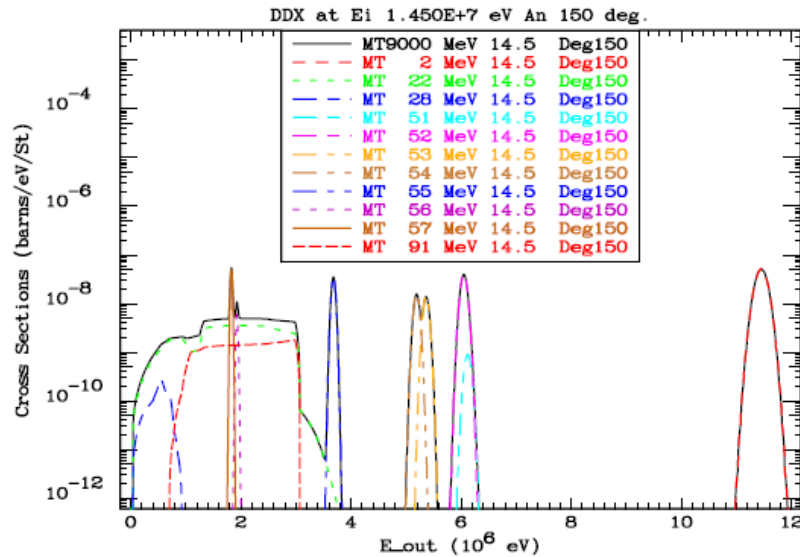


Figure. Contributions of various nuclear-data observables to the double-differential cross section at 14.5 MeV and 150° for ^{16}O

- ❑ This Figure shows the **DDXS at 14.5 MeV and 150° for ^{16}O of an infinitely thin sample**
- ❑ For the ^{16}O target, **continuum scattering** only contributes to the spectrum at very low outgoing-neutron energies, which agrees with the sensitivities of the ^{16}O spectra to MF=3, MT=91
- ❑ The pulsed-sphere spectrum is small in a comparable energy range and **several non-elastic channels** (MT=22, 56, 57) contribute to neutrons in the DDXS, making it hard to disentangle the effect of MT=91

Table: Those nuclear data that the calculated neutron-leakage spectra are sensitive to are listed by their MF and MT numbers for each pulsed sphere listed in Table 2. Only observables that have max. absolute sensitivities of approximately higher than 0.05 (%/%) are tabulated.

MF	1	3						4		5	6	
MT	452	2	4	16	18	>50	91	2	>50	18	16	91
Sphere	Isotopes to which the spectra are sensitive to											
Light water		¹ H		¹⁶ O	¹⁶ O		¹⁶ O	¹ H	¹⁶ O	¹⁶ O		
Heavy water		² H		¹⁶ O	¹⁶ O	² H		² H	¹⁶ O	¹⁶ O		² H
⁶ Li		⁶ Li	⁶ Li			⁶ Li		⁶ Li	⁶ Li			
Polyethylene		¹ H						¹ H				
Carbon		C	C			C	C	C	C			C
¹⁶ O		¹⁶ O	¹⁶ O			¹⁶ O	¹⁶ O	¹⁶ O	¹⁶ O			¹⁶ O
Concrete		¹ H						¹⁶ O	¹⁶ O			
		¹⁶ O	¹⁶ O			¹⁶ O		¹⁶ O	¹⁶ O			
		²⁸ Si	²⁸ Si			²⁸ Si		²⁸ Si	²⁸ Si			
Teflon		C	C			C		C	C			
		¹⁹ F	¹⁹ F			¹⁹ F		¹⁹ F	¹⁹ F			
Mg		²⁴ Mg	²⁴ Mg			²⁴ Mg	²⁴ Mg	²⁴ Mg	²⁴ Mg			²⁴ Mg
		²⁵ Mg	²⁵ Mg			²⁵ Mg	²⁵ Mg	²⁵ Mg				²⁵ Mg
		²⁶ Mg				²⁶ Mg						²⁶ Mg
²⁷ Al		²⁷ Al	²⁷ Al			²⁷ Al	²⁷ Al	²⁷ Al	²⁷ Al			²⁷ Al
Iron		⁵⁶ Fe	⁵⁶ Fe	⁵⁶ Fe		⁵⁶ Fe	⁵⁶ Fe	⁵⁶ Fe	⁵⁶ Fe			⁵⁶ Fe
		⁵⁶ Fe				⁵⁶ Fe		⁵⁶ Fe				⁵⁶ Fe
Lead		²⁰⁶ Pb	²⁰⁶ Pb	²⁰⁶ Pb		²⁰⁶ Pb	²⁰⁶ Pb	²⁰⁶ Pb	²⁰⁶ Pb			²⁰⁶ Pb
		²⁰⁷ Pb	²⁰⁷ Pb	²⁰⁷ Pb		²⁰⁷ Pb	²⁰⁷ Pb	²⁰⁷ Pb	²⁰⁷ Pb			²⁰⁷ Pb
		²⁰⁸ Pb	²⁰⁸ Pb	²⁰⁸ Pb		²⁰⁸ Pb	²⁰⁸ Pb	²⁰⁸ Pb	²⁰⁸ Pb			²⁰⁸ Pb
²³⁵ U	²³⁵ U	²³⁵ U	²³⁵ U		²³⁵ U	²³⁵ U	²³⁵ U	²³⁵ U	²³⁵ U	²³⁵ U		²³⁵ U
²³⁸ U	²³⁸ U	²³⁸ U	²³⁸ U		²³⁸ U	²³⁸ U	²³⁸ U	²³⁸ U	²³⁸ U	²³⁸ U		²³⁸ U
Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu		²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu	²³⁹ Pu		²³⁹ Pu

- The sensitivity analysis undertaken provided further guidance on which nuclear-data observables are contributing primarily to simulating pulsed-sphere spectra; this information is concisely summarized here.

Table: Those nuclear data in ENDF/B-VIII.0 that are recommended to be further investigated are identified by their MF and MT numbers.

Isotope	MF, MT of data recommended to be further investigated
⁶ Li	MF=3, MT={4, 51 - 90}; MF=4, MT={2, 51};
⁷ Li	MF=4, MT=2;
¹² C	MF=3, MT={4, > 50}; MF=4, MT={2, 51}; MF=6, MT=91;
¹⁶ O	MF=3, MT={2, 4}; MF=4, MT={2, 51}; MF=6, MT=91;
¹⁹ F	MF=3, MT={2, 4};
²⁴ Mg	MF=3, MT=2; MF=4, MT=2; MF=6, MT=91;
²⁵ Mg	MF=3, MT=91; MF=6, MT=91;
²⁶ Mg	MF=3, MT=2; MF=4, MT=2; MF=6, MT=91;
²⁷ Al	MF=3, MT=4; MF=4, MT=2; MF=6, MT=91;
⁴⁸ Ti	MF=3, MT=91; MF=4, MT=2; MF=6, MT=91;
⁵⁶ Fe	MF=3, MT={2, 4, 91}; MF=4, MT=2; MF=6, MT=91;
²⁰⁸ Pb	MF=3, MT={4, 91}; MF=6, MT={16, 91};
²³⁵ U	MF=1, MT=452; MF=3, MT={2, 4, 91}; MF=4, MT=2; MF=5, MT=18; MF=6, MT=91;
²³⁸ U	MF=3, MT={4, 91}; MF=4, MT=2; MF=5, MT=18; MF=6, MT=91;
²³⁹ Pu	MF=1, MT=452; MF=3, MT={18, 91}; MF=5, MT=18; MF=6, MT=91

- ❑ In this Table, those **nuclear-data observables are listed that are recommended to be further investigated** given the knowledge gained from studying biases in simulating LLNL pulsed spheres, sensitivity profiles and differential data
- ❑ These **suggestions are based on:**
 - 1) the analysis of simulated values and experimental data for the neutron-leakage spectra
 - 2) rough analysis of differential data available in EXFOR
 - 3) a sensitivity analysis highlighting to which nuclear data the neutron-leakage spectra are sensitive to

- ❑ **Important Benchmarks for ND validation... that are not yet in SINBAD**
 - LLNL pulsed spheres

- ❑ **Sensitivity Analysis using different techniques:**
 - MCSEN
 - SANDY and FRENDY

- ❑ **Sensitivity profiles for WPEC/SG47**
 - To extend sensitivities in other SINBAD benchmarks ?

- ❑ **Final comment**
 - *“Caution that not too strong conclusions should be drawn on the quality of nuclear data given the lack of UQ and Q&A on pulsed spheres”*
 - Forward Propagation: **“impact of nuclear data changes”** ... useful for ND evaluation
 - **Could NEA develop a new tool for SINBAD equivalent to NDaST code?**



Thank you for your attention!

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