

INDC(NDS)- 0694 Distr. FE, G

INDC International Nuclear Data Committee

Compensating Effects due to Nuclear Reactions and Material Cross Correlations in Integral Benchmarks

Summary Report from the Consultants Meeting

IAEA Headquarters 28 September – 1 October 2015

A.C. (Skip) Kahler Los Alamos National Laboratory, Los Alamos, NM, USA

> V. Pronyaev ATOMSTANDARD, Russia

A. Trkov Nuclear Data Section, IAEA, Vienna, Austria

January 2020

IAEA Nuclear Data Section Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from <u>http://www-nds.iaea.org/publications</u> or sent as an e-mail attachment. Requests for hardcopy or e-mail transmittal should be directed to <u>NDS.Contact-Point@iaea.org</u>

> or to: Nuclear Data Section International Atomic Energy Agency Vienna International Centre PO Box 100 1400 Vienna Austria

Printed by the IAEA in Austria

January 2020

INDC(NDS)- 0694 Distr. FE, G

Compensating Effects due to Nuclear Reactions and Material Cross Correlations in Integral Benchmarks

Summary Report from the Consultants Meeting

A.C. (Skip) Kahler

Los Alamos National Laboratory, Los Alamos, NM, USA

V. Pronyaev ATOMSTANDARD, Russia

A. Trkov Nuclear Data Section, IAEA, Vienna, Austria

January 2020

Contents

Introduction	7
Meeting Summary	8
Conclusions and Recommendations	9
Actions	10
Appendix I: Participants Summaries	11
Appendix II: Benchmark List	20
Appendix III Above-thermal Leakage Fractions for Thermal Solution Benchmarks	23
Appendix IV Agenda	25
Appendix V: List of Participants	27

Introduction Motivation and Objectives of the IAEA Consultants Meeting (CM)

The "Collaborative International Evaluated Library Organization (CIELO)" Pilot Program is a Working Party for Evaluation Cooperation (WPEC) Subgroup (SG40) sponsored by the Organization for Economic Development's (OECD) Nuclear Energy Agency (NEA).

SG40 is focused on developing evaluated nuclear data files for six nuclides $- {}^{1}$ H, 16 O, 56 Fe, 235,238 U and 239 Pu that represent a collective international consensus and would serve as candidate evaluations for use by the various regional evaluated nuclear data files (e.g., ENDF/B in the United States, JEFF in Europe, JENDL in Japan, etc).

The CIELO SG40 proposal, goals and objectives are available at <u>https://www.oecd-nea.org/science/wpec/sg40-cielo/SG40.pdf</u>. Of particular note in the CIELO SG40 proposal is

"... The goal is to provide evaluations that perform in integral simulations (k_{eff} , spectral indices, etc.) as well as, or better, compared to existing evaluations, whilst using more accurate fundamental cross sections and spectra data. CIELO data will not be adjusted in the formal sense, but we recognize that some aspects of CIELO will include evaluation choices based upon feedback from simulations of integral experiments. ..."

Since data testing of CIELO candidate evaluations may influence the content of those evaluations, the IAEA has convened a Consultant's Meeting to address this issue. Specifically, goals of this Consultant's Meeting are to (i) address compensating effects between different cross sections within a given evaluation as well as between different materials components within the integral benchmarks, and (ii) determine a suitable set of benchmarks to test the various candidate CIELO evaluations.

Further details on the Meeting can be found on the web page: <u>https://www-nds.iaea.org/index-meeting-crp/CM_Compensating_Effects_2015/</u>

Meeting Summary

The meeting opened with individual participant presentations, provided in Section 3, followed by detailed discussions on a potential strategy for selecting an appropriate set of benchmarks to satisfy the meeting objectives. These presentations provided an overview of current benchmark data testing practices.

Often benchmark testing at the participant institutions utilize a selection of benchmarks that have been developed over a period of years. The selection process is often ad hoc, being based upon "expert judgement", "experience", "intuition" or as a result of informal discussions among colleagues. However, as various benchmark databases have grown in size (for example, as of this writing the International Criticality Safety Benchmark Evaluation Project (ICSBEP) database contains over 550 evaluations and nearly 5000 experiments) it is not practical for any individual or committee to remain aware of all possible relevant benchmarks for a given application.

The OECD/NEA Data Bank has developed, and continues to develop, search tools that represent an important and useful means to sort the large collection of ICSBEP benchmarks which are a primary source of integral data for testing the various CIELO candidate evaluated data files.

Among the Data Bank products are "DICE" which can be used to obtain sensitivity information for most, currently about 80%, of the ICSBEP benchmarks. Another tool, "NDaST" uses these sensitivity data to assess the impact of cross section perturbations on integral benchmark parameters. These tools provide an efficient mechanism for selecting suitable benchmarks for more detailed simulation studies.

The participants of this CM strongly endorse the continued development of additional capabilities in these tools by the NEA. Specific capabilities that were mentioned during the CM participant discussions were to provide sensitivities to P_1 and P_2 Legendre scattering coefficients, to the prompt fission neutron spectrum (PFNS) and to reaction rates in these tools by the NEA.

During the various presentations and subsequent discussion, a number of key points were identified. These points can be summarized as

- Data adjustments based on integral experiments should not compromise the good physics and microscopic experimental data used to develop the evaluated nuclear data files.
- Data testing should start with "clean" benchmarks such as bare critical assemblies.
- Data testing should systematically be extended to benchmarks of added complexity, such as those that include reflected systems and/or mixtures of fissile, fertile and inert materials in the fuel region.
- Data testing should also include "clean" thermal benchmark systems such as solution systems and simple lattice configurations.
- Participants recognize that the transition from "fast" to "thermal" is more problematic with fewer clean benchmarks available. A more comprehensive study of the available benchmark databases utilizing the newly developed NEA tools would be appropriate.

Benchmarks used by the CM participants that may be useful are noted in Appendix II. Note that this list is primarily based upon the collective wisdom of the meeting participants. It is anticipated that as the technical community becomes more familiar with the NEA search tools noted above that changes, both additions and deletions, to this list will occur.

Data testers of CIELO candidate evaluations, and readers of the report, are reminded that the CIELO pilot project is limited in scope to a few specific nuclides, namely ¹H, ¹⁶O, ⁵⁶Fe, ^{235,238}U and ²³⁹Pu. As such, benchmarks that are poorly calculated due to deficiencies in the nuclear data of non-CIELO nuclides or for other unknown reasons should not, and will not, be fixed by the improved CIELO files. This caution is particularly relevant for benchmarks with significant quantities of iron or steel. CIELO's ⁵⁶Fe is only the dominant isotope by abundance and is not necessarily the dominant isotope responsible for possible discrepancies between calculated and measured parameters in integral benchmarks.

Conclusions and Recommendations

A strategy for addressing compensating effects, using the NEA DICE and NDaST tools, has been identified. The participants recognize the importance of these tools and endorse their continued development by the NEA.

The focus of the present work was on criticality benchmarks, but the participants acknowledge that other benchmark databases (IRPhEP, SINBAD and SFCOMPO, for example) should be considered.

A proposed categorization of potential criticality benchmarks has been developed. These categories include

- 1a. bare, fast critical assemblies containing 235 U
- 1b. bare, fast critical assemblies containing ²³⁹Pu
- 2a. ²³⁸U reflected, fast and intermediate critical assemblies containing ²³⁵U
- 2b. ²³⁸U reflected, fast and intermediate critical assemblies containing ²³⁹Pu
- 3a. Fe/SS reflected, fast and intermediate critical assemblies containing ²³⁵U
- 3b. Fe/SS reflected, fast and intermediate critical assemblies containing ²³⁹Pu
- 4a. other reflected, fast and intermediate critical assemblies containing 235 U
- 4b. other reflected, fast and intermediate critical assemblies containing ²³⁹Pu
- 5a. thermal critical assemblies (solutions and lattices) containing 235 U
- 5b. thermal critical assemblies (solutions and lattices) containing ²³⁹Pu or MOX

Reaction rate ratios should also be analyzed when available.

It is recommended that future CIELO meetings refer to the conclusions and recommendations of this Consultancy Meeting.

Actions

- 1. IAEA: will collect MCNP inputs contributed by the participant and make them available through the IAEA web site
- 2. Kahler: will create independent LCT42 models and contribute to IAEA
- 3. Trkov and Kahler: will compare LCT8 & LCT42 results
- 4. Bernard: will check if better MCNP and TRIPOLI CALIBAN inputs can be released; also provide latest CEA bias estimate (JEFF-3.1.1)
- 5. Go Chiba: attempt to prepare/release suitable MCNP input decks; development of MCNP models for the FCA-IX assemblies are desirable, since this benchmark addresses the sodium void coefficient. Future use of this assembly for CIELO testing will be limited until such models become available.
- 6. NEA Data Bank: will work on the implementation of extensions to the DICE and NDaST tools to provide more sensitivities to P₁ and P₂ Legendre scattering coefficients, PFNS and reaction rates.
- 7. Kahler: will provide ATLF and Average Energy of Lethargy causing Fission (EALF) for selected benchmarks.
- 8. All: reactivity calculations with ZPR-6/10 and Cu reflected benchmarks appear discrepant and need further investigation.
- 9. Cabello's /NEA: will make available Pronyaev's observations on the impact of detailed angular distributions on reactivity calculations to SG35.

Appendix I: Participants Summaries

CM participant summary discussions follow.

D. Bernard

"Decompensating Effects in Nuclear Data Integral Benchmarking"

Initially (2012), a project-based study was done within the framework of the OECD/NEA Uncertainty Analysis and Modelling for LWR [1]. The goal was to estimate integral parameter uncertainties (ND in particular) for LWR calculations (including neutronic and thermal-hydraulic physics). A specific parameter was the core power map, or the assembly power peaks in a large commercial LWR as GEN-III. After choosing available covariance matrices (COMMARA [2] or else), the major component of uncertainty (85% of the overall uncertainty) is due to ²³⁸U(n,n') cross section. To reach the target accuracy for LWR power map (and consequently the one for the control rod reactivity worth) implies a reduction by a factor 5 of the *a priori* covariance matrix for this particular cross section set. The need for this reduction was already shown for FBR applications (see HPRL [3]).

A first attempt [4] shown here is to interpret targeted ICSBEP benchmarks to validate this inelastic cross section. Natural uranium is often used in ICSBEP benchmarks. The interpretation of the reflector saving by comparing k_{eff} between bare geometry and reflected geometries allows us to validate the scattering cross sections of ²³⁸U. Indeed, one can show by equivalent first order standard perturbation theory that the sensitivity is maximal for inelastic reactions. This perturbation technique is very accurate because the reactivity worth associated with technological uncertainties is low. A second important parameter are spectral indices such as ²³⁵U(n,f)/²³⁸U(n,f) indicating the neutron slowing down and PFNS. After calculating Monte Carlo sensitivity of k_{eff}, reflector saving, spectral indices, to ^{235,238}U cross sections, one can estimate the following trend by maximizing the likelihood (Generalized least square method): the ²³⁸U(n,n') cross sections in JEFF-3.1.1 seems to be overestimated by about (11±3)%, especially the scattering to the continuum for 2 to 5MeV incident neutrons. This trend is independent of the *a priori* covariance matrix used, and a *posteriori* uncertainty is reduced by a factor of 5. This allows us to believe into this overestimation.

The second part of the talk is dedicated to the needed confirmation of this trend by performing a new experiment named EXCALIBUR@CALIBAN [5]. The principle of the experiment done in 2014 was to measure neutron flux transmissions (see [6]) through 1 sphere (phase 1) and through 2 cylinders (phase 2) by dosimetric activities. Finally, 75 transmission values were obtained within approximatively 3% of experimental uncertainty for the main transmissions corresponding to the plateau of ²³⁸U inelastic cross section. The interpretation with Monte Carlo codes of this experiment is planned for the end of 2016. This particular experiment is not sensitive to elastic scattering of ²³⁸U nor CALIBAN neutron spectrum (and hence to ²³⁵U PFNS) and will permit us to tag the inelastically scattered neutron by ²³⁸U.

The last part of the presentation is dedicated to some examples of inherent compensating effects in the integral analysis. Indeed, PFNS should be part of the analysis especially for high leakage experiment (regardless of whether the system is thermal or fast). Considering a fixed 60cm2 migration area for fast neutron, the k_{eff} sensitivity to leakage is a function of the dimension 'd' of the system (extrapolated dimension, in the sense of the neutron flux attenuation) through the simple formula: $k_{eff}=k_{inf}/(1+M^2xB^2)$ with $B^2=\pi/d^2$. The larger the system is (high 'd'), lower is the sensitivity of the k_{eff} to migration area. The latter could be estimated as the ratio between scattering diffusion coefficient and absorption coefficient. The fast neutron diffusion coefficient (leakage) can be consider as the product of elastic and inelastic (if any) cross sections and PFNS, thus explaining the possible confusion of wrong h or K1 extracted values (made of nubar, capture, and fission XS) in interpreting k_{eff} for small critical systems. For instance a high K1 value for a given fissile isotope which is obtained from integral small critical systems comparison between calculated k_{eff} and critical value could indicate that the PFNS used in the

calculation is harder than the actual one or because of a too small inelastic scattering at high energy (if its sensitivity is not negligible of course).

A final recommendation is to find a way to tag a specific cross section. For example, inelastic cross sections can be tagged by using transmission experiments or by adding incrementally a specific isotope and interpreting reactivity effect as a first order perturbation of the critical initial system (e.g. a reflected system versus bare system) thus avoiding a part of the technological uncertainty in benchmarking. Equally important is to produce an ENDF file with reduced and reliable covariance matrices.

Bernard References:

[1] https://www.oecd-nea.org/science/wprs/egrsltb/UAM/

[2] M. Herman et al., "COMMARA-2.0 Neutron Cross Section Covariance Library", BNL- 94830-2011 report

[3] <u>https://www.oecd-nea.org/dbdata/hprl/</u>

[4] A. Santamarina, D. Bernard, P. Leconte, J-F. Vidal, « Improvement of ²³⁸U Inelastic Scattering Cross-Section for an Accurate Calculation of Large Commercial Reactors », Proc. Of Int. Conf. ND2007

[5] D. Bernard, P. Leconte et al., « EXCALIBUR@CALIBAN: a neutron transmission experiment for ²³⁸U(n,n'_{continuum}g) nuclear data validation», Proc. Of Int. Conf, ANIMMA2013 (to be published in IEEE Transactions)

[6] H. Bethe et al., "Inelastic cross-sections for fissions-spectrum neutrons I", Journal of Nuclear Energy 1956, **Vol. 3**, *pp207-223* and following parts II-III and IV.

Bernard Benchmarks used in this study:

HMF-01, HMF-02, HMF-28, PMF-01, PMF-06, PMF-10, PMF-20, PMF-22, PMF-41, IMF-007, SCHERZO = SNEAK8= MINERVE k_{inf} "measured" values

<u>G.Chiba</u>

Firstly, benchmark calculation results of the CIELO test files are provided. Criticality data and spectral indices data of several fast neutron systems such as Godiva, Jezebel and Flattop are concerned. In addition, the FCA IX benchmark model, which has just been released by Dr. Fukushima of Japan Atomic Energy Agency, is also concerned. Usefulness of the FCA IX benchmark data for testing uranium-235 reaction cross sections in fast and intermediate energy ranges and uranium-235 PFNS are demonstrated. Results of sensitivity analyses to show a change of which nuclear data contributes to a change in integral quantity are also presented. Secondly, a result of an exercise of nuclear data adjustment for fast neutron energy range is presented. Three different sets of cross sections are used as an original nuclear data. Integral quantities are well reproduced by the adjusted nuclear data regardless of the original data, but the adjusted cross sections are significantly dependent on the original data. The detail will be given in the following section in this report. Finally, a new technique based on sub-space decomposition method is proposed in order to well understand the compensating effect. The singular value decomposition technique is applied to a sensitivity matrix, and then an orthonormal basis for a "sensitivity sub-space" is constructed. This decomposition gives some insights on the compensating effect. The detail also will be given in the following section.

Application of sub-space decomposition method to integral data testing

There are more than 1,000 criticality cases in the ICSBEP handbook, and the number of integral data sets increases if we consider other neutronics parameters such as spectral indices and other integral data base such as the IRPhEP handbook. The best way of the integral data testing is to use all of these integral benchmarks, but it is time-consuming and impractical. Among these existing integral data bases, a number of similar integral data, which have similar sensitivity profiles with each other, might

exist, so it is beneficial to develop a method to extract useful integral data from the huge-sized integral data base.

To identify the compensating effect in given integral data base is also an important issue. It might give beneficial insights on the compensating effect to know which nuclear data can be validated from the integral data base without any correlations with other nuclear data.

In order to address the above issues, a mathematical technique based on the sub-space decomposition method is proposed here.

Let us consider *a nuclear data space* spanned by an orthonormal set of nuclear data vectors. A sensitivity of one integral data with respect to nuclear data is defined as a vector in this nuclear data vector. If we have two nuclear data, σ_1 , σ_2 , for example, the dimension of this nuclear data space is two and a sensitivity of one integral data p with respect to nuclear data is described as a vector

$$\left(\frac{\mathrm{dp}}{\mathrm{d}\sigma_1}\cdot\frac{\sigma_1}{\mathrm{p}},\frac{\mathrm{dp}}{\mathrm{d}\sigma_2}\cdot\frac{\sigma_2}{\mathrm{p}}\right).$$

Let us assume that we have several integral data. Generally, the number of integral data is much smaller than the number of nuclear data, thus the space spanned by a set of sensitivity vectors is a sub-space of the nuclear data space. We will refer to this sub-space as *a sensitivity sub-space*.

If a nuclear data vector is in the sensitivity sub-space, this nuclear data vector can be reconstructed by a combination of nuclear data vectors. It means that this nuclear data can be independently validated by benchmark calculations with the set of the integral data and that this nuclear data is free from the compensating effect. On the other hand, a nuclear data vector is orthogonal to the sensitivity sub-space, this nuclear data cannot be validated with the set of integral data. We can quantitatively know how free the nuclear data is from the compensating effect by observing the Euclidean norm of a projected nuclear data vector on the sensitivity sub-space. Since nuclear data vector is a unit vector, the nuclear data is free from the compensating effect if the Euclidean norm of the projected vector is unity.

In order to construct the sensitivity sub-space from a set of sensitivity vectors, the singular value decomposition (SVD) technique is quite useful since the orthonormal set of vectors spanning the sensitivity sub-space can be automatically generated. A set of sensitivities can be described by a sensitivity matrix $\mathbf{S} = (\mathbf{s}_1, \mathbf{s}_2, ...)$, where \mathbf{s}_i is a sensitivity vector of the *i*th integral data. The SVD to this sensitivity matrix results in the following equations:

$\mathbf{S} = \mathbf{U}\mathbf{D}\mathbf{V}^{\mathrm{T}},$

where $\mathbf{D} = \text{diag}(v_1, v_2, ...)$ where v_i is the *i*th singular value. The so-called left-hand singular matrix $\mathbf{U} = (\mathbf{u}_1, \mathbf{u}_2, ...)$ is composed of the left-hand singular vectors \mathbf{u}_i . An orthonormal set of vectors $\mathbf{S} = \{\mathbf{u}_1, \mathbf{u}_2, ...\}$ spans the sensitivity sub-space. In the SVD, we have to set a threshold value for singular values because a vector corresponding to small singular value should be discarded in actual application.

Let us consider that we have some integral data and try to add other integral data to the original data base. In that case, it is important to know whether the addition of these new integral data is effective or not. We can answer to this question by comparing dimensions of the sensitivity sub spaces (the number of non-negligible singular values) before and after the new integral data addition. If dimensions of the sensitivity sub-space increases, the additional integral data can contribute to increase the effectiveness of the set of integral data for nuclear data validation. In this moment, we do not consider benchmark uncertainty, so this should be considered somehow in the actual applications.

The left-hand singular vectors might be useful to consider the compensating effect because inter-nuclear data dependence is described.

The orthogonal projection of a unit nuclear data vector to the sensitivity sub-space can be done as follows. Let us consider the *j*th nuclear data described as a unit vector \mathbf{e}_j . The projected vector to the sensitivity sub-space, \mathbf{e}'_j , can be written as

$$\mathbf{e}_{j}^{\prime}=\mathbf{P}_{\mathrm{U}}\mathbf{e}_{j},$$

where $\mathbf{P}_{\mathbf{U}} = \mathbf{U}\mathbf{U}^{\mathrm{T}}$. Let us be reminded that **U** is a left-hand singular matrix. The Euclidean norm of \mathbf{e}'_{j} , $\|\mathbf{e}'_{i}\|$, can be a good measure to know how free the jth nuclear data from the compensating effect.

Exercise of nuclear data adjustment with integral data sensitive to fast energy range

Generally, the number of integral data is much smaller than the number of nuclear data if neutron energy is discretized to several dozens of groups or more. Thus, there is no unique nuclear data to perfectly reproduce the integral data. The so-called nuclear data adjustment technique produces a unique nuclear data by maximizing likelihood of the conditional probability distribution on nuclear data. This is just a mathematical procedure, and the obtained nuclear data, i.e., adjusted nuclear data, might significantly depend on the prior covariance data, the prior cross section and the sensitivity profiles. One has to be careful when observing the adjusted cross section. It gives some insights on further nuclear data improvement, but it does NOT provide any information on the true values of cross section.

To confirm the above, results of a simple exercise of nuclear data adjustment is described here. Only fast neutron energy is concerned in this exercise and the following 23 integral data; 14 of them are criticality data and others are spectral indices data. The list of the used integral data is shown below:

Index	Name	
1	Jezebel	
2	Jezebel-Pu	
3	Jezebel-233	
4	Godiva	
5	Flattop-Pu	
6	Flattop-U	
7	Flattop-233	
8	Big-ten	
9	Thor	HEU with Th reflector
10	PMF010	Pu with NU reflector
11	U3MF002-1	U3 with HEU reflector
12	U3MF002-2	U3 with HEU reflector
13	U3MF003-1	U3 with NU reflector
14	U3MF003-2	U3 with NU reflector
15	F8/F5 in Jezebel	
16	F3/F5 in Jezebel	
17	F9/F5 in Jezebel	
18	F8/F5 in Godiva	
19	F3/F5 in Godiva	
20	F9/F5 in Godiva	
21	F8/F5 in Jezebel-233	
22	F3/F5 in Jezebel-233	
23	F9/F5 in Jezebel-233	

Three different sets of 70-group cross sections are prepared from ENDF/B-VII.1. JENDL-4.0 and JEFF-3.2, and these original cross section sets are adjusted by using the 23-integral data. Sensitivity profiles of the integral data with respect to nuclear data are calculated by a deterministic reactor physics code system CBZ being developed at Hokkaido University, Japan. Note that common cross section covariance data based on JENDL-4.0 is used since ENDF/B-VII.1 and JEFF-3.2 do not contain covariance data for elastic scattering angular distribution (MF34) which is quite important in fast neutron systems.









By the nuclear data adjustment, C/E values become close to unity regardless of the original cross section data.

The following figures are comparisons of cross sections before and after the adjustment:





As shown in the above figures, the adjusted cross sections are quite different from each other even each set of the cross sections give similar results on the integral quantities.

These results clearly show that there is a compensating effect in the adjusted cross sections and that the adjusted cross section does NOT provide any information on true values of cross sections.

V Pronyaev

Strategy of compensating effects excluding from major fissile (²³⁵U, ²³⁹Pu), fertile (²³⁸U), moderating (H, O, C) and structural (⁵⁶Fe) materials

General principles:

- 1. use only "clean" benchmarks (benchmarks, which mostly includes the studied materials and insensitive to all other)
- 2. use modern evaluations of PFN which give approximately 1.5% (mean energy) softer spectrum, than previous evaluations. The uncertainty in the mean energy is between 0.2 0.5%.
- 3. stay well in the limits of low uncertainties for standards and other recommended reactions cross sections and parameters
- 4. begin with single fissile material benchmarks and resolve the compensating effects between reactions of this material, using not only k_{eff} benchmarks but also measured reaction rates (usually ratio to ²³⁵U(n,f)), transmissions and some other integral experimental parameters
- 5. move to two-material benchmarks (fissile (²³⁵U and ²³⁹Pu)+fertile material (²³⁸U))
- 6. move to waters solutions of large assemblies with low concentration of fissile material and well determined thermal values of the cross sections and PFNS and adjust Hydrogen capture if needed. Elastic cross section at Hydrogen is a primary standard and is known within 0.3% uncertainty. Sensitivity to Oxygen cross sections is negligible

The same experiment (different cases) when one varied quantity which influence much of the spectrum in the system

Benchmark HMF007 is very important from this point of view.

Instrumentation:

Start from NDaST for effective analysis using sensitivities and perturbations

After possible indication at the resolving the problem, finalize by changing the evaluation and using MC calculations

List of benchmarks for adjusting of cross sections and constants

²³⁵U high enriched water solutions thermal (HST)

4 benchmarks which were used for K1 parameter determination:

HST013-1 (large sphere)

HST032 (large sphere)

HST042-1 (large cylinder)

HST042-8 (large cylinder)

allow minor adjustments of nu-bar, fission and capture cross section at thermal point and capture cross section at Hydrogen. Practically insensitive to the Oxygen

Assembly	nu-bar (²³⁵ U)	Fission (²³⁵ U)	Capture (²³⁵ U)	Capture (¹ H)	Elastic (¹ H)		mu-bar (¹ H)	
	integral	integral	integral	integral	integral	Above 100 keV	integral	Above 100 keV
HST013-1	1.0000	0.5100	-0.0867	-0.3938	0.2692	0.2000	-0.1380	-0.1000
HST032	0.9997	0.5601	-0.0778	-0.4716	0.1097	0.0800	-0.0520	-0.0400
HST042-1	1.0000	0.5736	-0.0816	-0.4330	0.1872	0.1500	-0.0916	-0.0800
HST042-8	0.9960	0.5789	-0.0733	-0.4993	0.0274	0.0180	-0.0100	-0.0080

Major sensitivities

Appendix II: Benchmark List

A selection of benchmarks used or recommended for use by the CM participants is itemized in the Table. The benchmark list is order by the category definitions provided in the main body of this document.

1a. bare, fast critical assemblies containing ²³⁵U

Several benchmarks are available in the ICSBEP database.

No. ICSBEP label Short name Common name

1	HEU-MET-FAST-001	hmf001	Godiva
2	HEU-MET-FAST-008	hmf008	VNIIEF-CTF-bare
3	HEU-MET-FAST-015	hmf015	VNIIEF-CTF-UnrCy1
4	HEU-MET-FAST-065	hmf065	VNIIEF-CTF-UnrCy2
5	HEU-MET-FAST-018	hmf018	VNIIEF_Sphere
6	HEU-MET-FAST-051	hmf051-01	ORCEF-01
7	HEU-MET-FAST-051	hmf051-02	ORCEF-02
8	HEU-MET-FAST-051	hmf051-03	ORCEF-03
9	HEU-MET-FAST-051	hmf051-15	ORCEF-15
10	HEU-MET-FAST-051	hmf051-16	ORCEF-16
11	HEU-MET-FAST-051	hmf051-17	ORCEF-17
12	HEU-MET-FAST-100	hmf100-1	ORSphere-1
13	HEU-MET-FAST-100	hmf100-2	ORSphere-2
14	HEU-MET-FAST-080	hmf080	Caliban

1b. bare, fast critical assemblies containing ²³⁹Pu

The equivalent bare assemblies with a plutonium core are rare.

No. ICSBEP label Short name Common name

1	-	PU-MET-FAST-001	pmf001	Jezebel	
2	2	PU-MET-FAST-001	pmf001-001d	Jezebel-1	(detailed)
3	3	PU-MET-FAST-001	pmf001-002d	Jezebel-2	(detailed)
4	l	PU-MET-FAST-001	pmf001-003d	Jezebel-3	(detailed)
5	5	PU-MET-FAST-001	pmf001-004d	Jezebel-4	(detailed)
6	5	PU-MET-FAST-002	pmf002	Jezebel-24	0
7	7	PU-MET-FAST-022	pmf022	pmf022	
8	3	PU-MET-FAST-029	pmf029	pmf029	

2. ²³⁸U reflected and intermediate-enriched, fast and intermediate-spectrum critical assemblies containing ²³⁵U and ²³⁹Pu

The list below includes some of the commonly used benchmarks to validate the data in the fast and intermediate energy range.

No. ICSBEP label Short name Common name

1	HEU-MET-FAST-001	hmf001	Godiva
2	HEU-MET-FAST-028	hmf028	Flattop-25
3	IEU-MET-FAST-007	imf007d	Big_Ten(detailed)
4	PU-MET-FAST-001	pmf001	Jezebel
5	PU-MET-FAST-002	pmf002	Jezebel-240
6	PU-MET-FAST-006	pmf006	Flattop-Pu
7	U233-MET-FAST-001	umf001	Jezebel-U233
8	U233-MET-FAST-006	umf006	Flattop-23
9	PU-MET-FAST-022	pmf022	Bare(98
10	PU-MET-FAST-029	pmf029	Bare(88
11	IEU-MET-FAST-001	imf001-001	Jemima-1
12	IEU-MET-FAST-001	imf001-002	Jemima-2
13	IEU-MET-FAST-001	imf001-003	Jemima-3
14	IEU-MET-FAST-001	imf001-004	Jemima-4

3. Fe/SS reflected, fast and intermediate critical assemblies containing 235 U and 239 Pu

The list is based on sensitivities obtained from the DICE sustem from the NEA Data bank but is there might be other benchmarks that are also sensitive to iron data.

1	HEU-MET-FAST-013	hmf013	VNIITF-CTF-SS-13
2	HEU-MET-FAST-021	hmf021	VNIITF-CTF-SS-21
3	HEU-MET-FAST-024	hmf024	VNIITF-CTF-SS-24
4	HEU-MET-FAST-087	hmf087	VNIITF-CTF-Fe
5	HEU-MET-FAST-088	hmf088-1	hmf088-1
6	HEU-MET-FAST-088	hmf088-2	hmf088-2
7	HEU-MET-INTER-001	hmi001	ZPR-9/34
8	HEU-MET-THERM-013	hmt013-2	Planet Fe-2
9	HEU-MET-THERM-015	hmt015	—
10	IEU-MET-FAST-005	imf005	VNIIEF-CTF-5
11	IEU-MET-FAST-006	imf006	VNIIEF-CTF-6
12	LEU-COMP-THERM-042	lct042-1	lct042-1
13	LEU-COMP-THERM-042	lct042-2	lct042-2
14	LEU-COMP-THERM-043	lct043-2	IPEN/MB-01
15	LEU-MET-THERM-015	lmt015	RB-Vinca(15)
16	MIX-COMP-FAST-001	mcf001	ZPR-6/7
17	MIX-COMP-FAST-005	mcf005-s	ZPR-9/31
18	MIX-COMP-FAST-006	mcf006-s	ZPPR-2
19	PU-MET-FAST-015	pmf015	BR-1-3
20	PU-MET-FAST-025	pmf025	pmf025
21	PU-MET-FAST-026	pmf026	pmf026
22	PU-MET-FAST-028	pmf028	pmf028
23	PU-MET-FAST-032	pmf032	pmf032
24	PU-MET-INTER-002	pmi002	ZPR-6/10
25	PU-MET-INTER-003	pmi003-001s	ZPR-3/58(U)
26	PU-MET-INTER-004	pmi004-001s	ZPR-4/59(Pb)
27	IEU-COMP-INTER-005	_ ici005	ZPR-6/6A

No. ICSBEP label Short name Common name

4. Other reflected, fast and intermediate critical assemblies containing ²³⁵U

Other benchmarks are still to be identified and agreed upon.

5. Thermal solution critical assemblies containing ²³⁵U

The short list, which is reasonably representative of the longer list commonly used at LANL is given below. A short list of plutonium solution benchmarks is not yet established.

No. ICSBEP label Short name Common name

1	HEU-SOL-THERM-009	hst009-1	ORNL_S1	
2	HEU-SOL-THERM-009	hst009-4	ORNL S4	
3	HEU-SOL-THERM-013	hst013-1	ORNL T1	
4	HEU-SOL-THERM-032	hst032	ORNL T5	
5	HEU-SOL-THERM-001	hst001-04	R04	
6	HEU-SOL-THERM-001	hst001-05	R05	
7	HEU-SOL-THERM-001	hst001-07	R07	
8	HEU-SOL-THERM-042	hst042-1	ORNL C1	
9	HEU-SOL-THERM-042	hst042-4	ORNLC4	
10	HEU-SOL-THERM-042	hst042-8	ORNLC8	
11	HEU-SOL-THERM-043	hst043-003	ORNL_LS3	
12	HEU-SOL-THERM-010	hst010-1	ORNL S10T0	
13	HEU-SOL-THERM-012	hst012	ORNL_S91	
			—	

Appendix III Above-thermal Leakage Fractions for Thermal Solution Benchmarks

The above-thermal leakage fractions for selected thermal solution benchmarks were provided by A. Kahler.

		LOT Come		DOT O		DOT On a		DOT O	
HST.Case HST1 1	ATLF 0.420153	LST.Case	0 201669	PST.Case PST1_1	ATLF 0.460603	PST.Case PST7 10	0 476126	PST.Case PST22.1	ATLF 0 340343
HST1 2	0.420100	1 ST4 2	0.188173	PST1 2	0.470266	PST0 33	0.056304	PST22.1	0.334416
HST1 3	0.444000	LOT4.2	0.100173	PST1 3	0.47/0200	PST10.1	0.030304	PST22.2	0.315777
	0.412122		0.160220	DST1 4	0.491200	PST10.2	0.467472	DST22.0	0.302417
HST1 5	0.338001	LS14.4	0.100230	PST1.4	0.401200	PST10.2	0.407473	PST22.4	0.302417
	0.330331		0.141164	DST1.6	0.473035	PST10.4	0.422491	DST22.0	0.269630
LIGT1 7	0.347421	1974.0	0.141104	PST1.0	0.404040	PST10.4	0.432401	PGT22.0	0.209030
	0.404004		0.100400		0.439142	PST10.5	0.419702	POT22.7	0.259471
	0.421234		0.190429	PS12.2	0.440460	PST 10.6	0.431931	PS122.0	0.250008
	0.250440	LO17.2	0.175923	PS12.3	0.440003	PST 10.7	0.419463	PS122.9	0.241833
	0.309449	LS17.3	0.101322	PS12.4	0.451011	PST 10.8	0.399035	PO120.1	0.391000
	0.502525	LOT7.6	0.147010	PS12.0	0.452072	PS110.9	0.433009	PO120.2	0.303773
HST0.2	0.563539	LS17.5	0.137636	PS12.0	0.462000	PST10.10	0.436609	PS120.3	0.376694
HST0 4	0.559993	LST20.1	0.152623	PS12.7	0.403/02	PST10.11	0.434009	PS128.4	0.300147
HST40.4	0.046797	LST20.2	0.130107	PS13.1	0.401177	PST10.12	0.419561	PS120.5	0.336064
	0.490473	LST20.3	0.113573	PS13.2	0.404397	PST10.13	0.390200	PS120.0	0.333037
	0.412000	LST20.4	0.096964	PS13.3	0.400432	PST10.14	0.377113	PS120.7	0.482008
	0.2066.47		0.144725	PS13.4	0.407549	PST11.18.1	0.277401	PS120.0	0.4/3/18
HOT12	0.200047	LOT21.2	0.120395	PS13.0	0.413130	PST11.10.2	0.270925	PS120.9	0.400411
цетаа	0.143747	LST21.3	0.100230	PS13.0	0.420225	PST11 19 /	0.270090	POT02.1	0.335050
LIST 12 1	0.000107	L3121.4	0.091391	PS13.7	0.417910	PST11 19 5	0.203029	PGT22.2	0.345051
LIST42.1	0.099000			PS13.0	0.419095	PST11 19 6	0.200000	PGT32.3	0.330417
HST42.2	0.054800			PS14.1	0.370139	PST11 19 7	0.292551	PGT22.5	0.327373
HST42.5	0.034035			PST4.2	0.371770	PST11.16.1	0.202020	PGT22.6	0.310001
HST42.4	0.036040			PS14.3	0.374331	PST11 16 2	0.320040	PST32.0	0.302303
HST42.5	0.020097			PS14.4	0.370022	PST11 16 2	0.320001	PGT22.0	0.293021
HST42.0	0.020332			PST4.5	0.372303	PST11 16 /	0.323503	PST32.0	0.202039
LIST42.7	0.009134			PS14.0	0.371409	PST11 16 5	0.333000	PGT22.9	0.264105
LIST42.0	0.003012			PS14.7	0.372110	PST12.1	0.343109	PGT22.10	0.204195
LIST43.1	0.423070			PST4.0	0.373923	PST12.1	0.173030	PGT22.11	0.250001
LIST43.2	0.130304			PST4.9	0.301304	PST12.2	0.122101	PGT22.12	0.202170
HQT50 1	0.142004			PST4.10	0.392002	PST12.5	0.100101	PGT22.13	0.393179
HST50.1	0.445639			PST4.11	0.404500	PST12.4	0.055555	PGT22.14	0.362702
HST50.2	0.449030			PST4.12	0.373027	PST12.5	0.000330	PGT22.15	0.309702
HST50.3	0.430040			PST5 1	0.372119	PST12.0	0.340700	PS132.10	0.334100
HST50.4	0.4447562			PS13.1	0.371903	PST12.7	0.342410	PGT24 1	0.340301
	0.447505			PST5 2	0.374192	PST12.0	0.310230	PS134.1	0.420090
HST50.0	0.442131			PST5.4	0.370071	PST12.9	0.237334	PS134.2	0.340347
	0.441222			PS15.4	0.301951	PST12.10	0.234903	PST34.3	0.230300
HST50.0	0.447037			PST5.6	0.305300	PST12.11	0.133402	PS134.4	0.239339
HST50.9	0.441407			PS15.0	0.350500	DQT12.12	0.173033	PGT24.0	0.150100
HOTEO 14	0.400017			PO10./	0.402//4	DQT10 1	0.000778	PO104.0	0.100102
n9190.11	0.431191			PO10.0	0.376040	DQT10.1	0.203004	PO104./	0.321903
				DOTE 4	0.3/0910	POT 10.2	0.2033/4	F 0 1 04.0	0.306917
				POTO 0	0.343104	FOI 10.3	0.204018	F3134.9	0.290930
				PO10.2	0.34/801	ГЭН 10.4 DOT10 F	0.202050	PO104.10	0.270034
				PO10.3	0.354159	POT 10.5	0.198943	PO134.11	0.200030
				P517.2	0.485/6/	PS118.6	0.192175	P5134.12	0.23/516

	PST7.3	0.489579	PST18.7	0.182618	PST34.13	0.219307
	PST7.5	0.473067	PST18.8	0.165689	PST34.14	0.203317
	PST7.6	0.477539	PST18.9	0.150354	PST34.15	0.193548
	PST7.7	0.475750			PST38.1	0.173416
	PST7.8	0.480613			PST38.2	0.178083
	PST7.9	0.481293			PST38.3	0.104818
					PST38.4	0.090430
					PST38.5	0.090661

Appendix IV Agenda

Consultants' Meeting on

"Compensating Effects due to Nuclear Reaction and

Material Cross Correlations in Integral Benchmarks"

IAEA Headquarters, Vienna, Austria 28 September – 1 October 2015

Meeting Room MOE60

AGENDA

Monday, 28 September

09:00 - 09:30 Registration (IAEA Registration desk, Gate 1)

09:30 - 10:15 Opening Session

Welcoming address and Introduction – Arjan Koning (IAEA-NDS Section Head) Election of Chairman and Rapporteur Adoption of Agenda Administrative matters

10:15 - 12:30 Presentations by participants (about 45 min each)

- 1. A. Trkov: Objectives of the CM on Compensating Effects due to Nuclear Reaction and Material Cross Correlations
- 2. D. Bernard: Decompensating effects in Nuclear Data integral benchmarking: how to tag a specific XS? Example of 238U(n,n') and 235U (or 239Pu) PFNS

Coffee break as needed

12:30 – 14:00 Lunch

14:00 – 17:30 Presentations by participants (cont'd)

- 3. O. Cabellos: NEA Activities and NEA Tools: A Bayesian Approach for Compensating Effects and Analysis of k_{eff} Sensitivity Profiles
- 4. I. Hill: (Included in the presentation by O. Cabellos)
- 5. A. Trkov: On the Compensating Effects in the Evaluated Cross Sections of ²³⁵U

Coffee break as needed

Tuesday, 29 September

09:00 - 12:30 **Presentations by participants (cont'd)**

- 6. A. Kahler: LANL Experience using ICSBEP Benchmarks for Cross Section Data Testing
- 7. Go Chiba:
 - a. Sensitivity analysis of CIELO test files for fast neutron systems
 - b. Exercise of nuclear data adjustment with fast neutron systems
 - c. Application of sub-space method for nuclear data validation
- 8. Liu Ping: Benchmarks for Data Testing of Iron

Coffee break as needed

12:30 – 14:00 Lunch

14:00 – 17:30 **Presentations by participants (cont'd)**

- 9. V. Pronyaev: Uncertainties of the Evaluated Nuclear Data and Compensation Effects in the Criticality
- 10. C. Lubitz: Compensating Effects in O16 and U235 (Cancelled)
- 15:30 17:30 Round Table Discussion

Coffee break as needed

Wednesday, 30 September

09:00 - 12:30 Round Table Discussion

- Strategy for dealing with compensating effects
- Use of sensitivities to identify suitable benchmarks
- Can a common list of suitable benchmarks be produced?

Coffee break as needed

- 12:30 14:00 Lunch
- 14:00 17:30 **Round table discussion (cont'd)**

Coffee break as needed

Thursday, 1 October

09:00 - 17:00 Drafting of the summary report

Coffee and lunch break(s) in between

17:00 Closing of the meeting

Appendix V: List of Participants

Consultants' Meeting on

"Compensating Effects due to Nuclear Reaction and Material Cross Correlations in Integral Benchmarks"

> IAEA, Vienna, Austria 28 September – 1 October 2015

LIST OF PARTICIPANTS

CHINA

Liu **Ping** China Nuclear Data Center China Institute of Atomic Energy P.O. Box 275 (41) 102413 Beijing Tel: + 86 10-6935-7712 E-mail: <u>ping@ciae.ac.cn</u>

FRANCE

Oscar **Cabellos** NEA Data Bank OECD Nuclear Energy Agency Le Seine Saint-Germain 12 boulevard des Iles 92130 Issy-les-Moulineaux Tel: + 33 1 45241084 E-mail: <u>oscar.cabellos@oecd.org</u>

David **Bernard** Centre d'Etudes Nucleaires de Cadarache Batiment 230 13108 Saint-Paul-lez-Durance Tel: +33 442254913

E-mail: david.bernard@cea.fr

JAPAN

Go **Chiba** Hokkaido University Graduate School of Engineering Kita 13-jo Nishi 8-chome Sapporo 060-8628 E-mail: <u>go_chiba@eng.hokudai.ac.jp</u>

USA

Albert **Kahler** Los Alamos National Laboratory Building 200, Room 215 P.O. Box 1663, MSB214 Los Alamos NM 87545 Tel: + 1 505 606 2042 E-mail: <u>akahler@lanl.gov</u>

Cecil Lubitz Knolls Atomic Power Laboratory (KAPL) P.O. Box 1072 Schenectady NY Tel: +

E-mail: clubitz@nycap.rr..com

RUSSIA

Vladimir **Proniaev** ATOMSTANDART ROSATOM State Corporation Bolshaya Ordynka str., 24 Moscow Tel: +7 9105166773 (Mobile) E-mail: <u>vgpronyaev@atomstandard.ru</u> <u>vgpronyaev@yandex.ru</u>

IAEA

Andrej **Trkov** International Atomic Energy Agency Nuclear Data Section Division of Physical and Chemical Sciences Wagramer Strasse 5 A-1400 Vienna Tel. +43-1-2600 21712 E-mail: <u>a.trkov@iaea.org</u>

Roberto Capote Noy

International Atomic Energy Agency Nuclear Data Section Division of Physical and Chemical Sciences Wagramer Strasse 5 A-1400 Vienna Tel. +43-1-2600 21713 E-mail: roberto.capotenoy@iaea.org

Nuclear Data Section International Atomic Energy Agency Vienna International Centre, P.O. Box 100 A-1400 Vienna, Austria E-mail: nds.contact-point@iaea.org Fax: (43-1) 26007 Telephone: (43-1) 2600 21725 Web: http://www-nds.iaea.org