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MCNP modelling of the ASPIS Iron88 SINBAD shielding benchmark

Bor Kos

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Ivan A. Kodeli

Jožef Stefan Institute
Ljubljana, Slovenia

September 2018

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

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POVZETEK:
V poročilu je opisan postopek modeliranja referenčnega eksperimenta ASPIS Iron88 z baze podatkov SINBAD za potrebe simuliranja transporta nevtronov s pomočjo programa MCNP. V prvem delu je predstavljena motivacija za modeliranje. Poročilo se nadaljuje z opisom modeliranja geometrije eksperimenta v CAD programu Rhinoceros, transformacija v geometrijski zapis formata MCNP. Podrobno je opisan tudi postopek modeliranja materialov, izvora in posameznih cenilk detektorjev. Sledi opis določevanja parametrov redukcije variance s pomočjo programa ADVANTG. V zadnjem delu poročila so navedeni rezultati primerjave eksperimentalnih rezultatov s simulacijami za pet različnih detektorjev (žveplo, indij, rodij, zlato, aluminij) s štirimi (ENDF/B-VII.1, ENDF/B-VIII, JEFF-3.3 and JENDL-4.0u) knjižnicami jedrskih podatkov. Rezultati z zlatimi aktivacijskimi folijami so na tej točki še preliminarni in zahtevajo dodatno občuljivostno študijo in se ne priporočajo za validacijo jedrskih podatkov (Na željo naročnika je poročilo podano v angleščini).

Ključne Besede: MCNP, ASPIS, ŽELEZO, ADVANTG, SINBAD

ABSTRACT:
The report describes the modelling procedure for MCNP of the ASPIS Iron88 shielding benchmark experiment form the SINBAD database. In the first part of the report motivation behind the modelling is given. The report continues with a detailed description of the geometrical properties of the benchmark with the Rhinoceros CAD program and the transformation procedure of the CAD model in to MCNP format. In the next part of the report details are given on the material, source and detector (tally) modelling of the benchmark experiment. Furthermore the variance reduction procedure using ADVANTG is described. Finally the results of the comparison of the experimental results to the calculation results for five different detectors (Sulphur, Indium, Rhodium, Gold, Aluminium) and with four different nuclear data libraries (ENDF/B-VII.1, ENDF/B-VIII, JEFF-3.3 and JENDL-4.0u) is given. Results for the Gold activation foils are only preliminary at this point and require an additional sensitivity study before they can be recommended for nuclear data validation applications.

Keywords: MCNP, ASPIS, IRON, ADVANTG, SINBAD

September 2018

Definition of Symbols, Terms and Abbreviations

IAEA	International Atomic Energy Agency
ASPIS	Shielding facility installed at the NESTOR reactor at Winfrith
SINBAD	Shielding Integral Benchmark Archive and Database
CIELO	Collaborative International Evaluated Library Organisation
MCNP	General purpose **M**onte **C**arlo **N**-**P**article transport code
ADVANTG	**A**utomate**D** **VA**ria**N**ce reduc**T**ion **G**enerator
CPU	Central Processing Unit
CAD	Computer Assisted Design
Rhino	Rhinoceros CAD software program
JSI	”Jožef Stefan” Institute
NIST	National Institute of Standards and Technology
ORNL	Oak Ridge National Laboratory
WW	Weight Window variance reduction parameters
FW-CADIS	Forward-Weighted Consistent Adjoint Driven Importance Sampling method
PFNS	Prompt fission neutron spectrum
C/E	Calculation-over-Experiment

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1 Introduction

The ASPIS Iron88 [1, 2, 3, 4] shielding experiment is one of several high quality experiments included in the SINBAD (Shielding Integral Benchmark Archive and Database) database [5, 6, 7, 8]. It includes experimental results for five different foil activation detectors (Sulphur, Indium, Rhodium, Gold and Aluminium) located at various thicknesses of mild-steel shields ranging from 5 cm to roughly 80 cm. The neutron source was produced by using the thermal neutrons form the NESTOR reactor to induce fission of ^{235}U in a fission plate.

The motivation behind the development of new MCNP [9] (General purpose **M**onte **C**arlo **N**-**P**article) models of the ASPIS Iron88 shielding benchmark experiment from the SINBAD database arises from the CIELO (Collaborative International Evaluated Library Organisation) project. The success and the controversy of the project was largely based on the fact that the benchmarking was an integral part of the evaluation process. In order for the benchmarks to be suitable for the validation and, eventually, evaluation processes they have to be of a high order of quality. The ASPIS experiments are of interest for evaluation purposes because of their fission energy neutron spectra and deep penetration examples with different integral activation (Sulphur, Indium, Rhodium, Gold and Aluminium) detectors. Effective variance reduction parameters for these models did not exist beforehand and were developed together with new geometrical models for each of the detectors.

Because this is a deep penetration shielding problem effective variance reduction parameters were needed for CPU (Central Processing Unit) time-wise effective calculations. The source was geometrically and energy biased and space and energy dependent weight window variance reduction parameters were produced using the ADVANTG [10] hybrid deterministic/Monte Carlo code.

In Section 1.1 of the report the contract details with IAEA (International Atomic Energy Agency) are given. Section 2 contains all of the modelling details, from the initial CAD (Computer Assisted Design) modelling (2.1), to the MCNP geometrical modelling (2.2), material (2.2.1) and source definition (2.2.2) to the detector/tally modelling (2.2.3). A separate Section (3) of the report is dedicated to the variance reduction techniques implemented. Open issues of the models are described in 4. References for the computer codes used for each of the modelling steps are given in appropriate sections of the report. Finally the results, namely Calculation-over-Experiment (C/E) results for the five different detectors (Sulphur 5.1, Indium 5.2, Rhodium 5.3, Gold 5.4 and Aluminium 5.5) calculated with MCNP5 ver. 1.6 and four different nuclear data libraries (ENDF/B-VII.1, ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0u) and the International Reactor Dosimetry and Fusion File IRDFF v.1.05 [11] are given in Section 5.

1.1 Deliverables according to contract

The deliverables according to the IAEA special service agreement (Requisition No: TAL-NAPC20180606-001) are:

"*MCNP input model for the ASPIS-88 iron benchmark, including some form of variance reduction that will allow execution of the test problem in reasonable time for all the activation monitors. Document describing the model, the variance reduction technique, and notes on any deficiencies in the specifications that might influence the results. The reports must include at least the results of sample calculations with the ENDF/B-VII.1 and ENDF/B-VIII libraries.*"

The deliverables can be broken in-to the following items:

- MCNP models including geometrical, source and tally definitions for the iron and concrete shielding cases
- Effective variance reduction parameters
- Document with detailed description of the modelling procedure
- Sample calculations with ENDF/B-VII.1 and ENDF/B-VIII nuclear data libraries

Items 1 and 2 will be delivered separately as MCNP input files (*.i) and external weight window files (*.wwinp). The list of all MCNP input files and weight window files is given in Appendix C. A sample input file is given in Appendix B. Items 3 and 4 are addressed in this report.

2 ASPIS Iron88

The ASPIS shielding tank was installed in one of the four experimental caves of the NESTOR light water cooled, graphite and light water moderated reactor at Winfrith. The experimental cave can be isolated from the reactor with a combination of neutron/gamma-ray shielding materials. Different shielding configurations can be installed vertically in a mobile tank with a surface of 1.8 m × 1.8 m and a length of 3.7 m. Thermal neutrons from the outer graphite reflector of the NESTOR reactor are used to drive a fission plate placed in the ASPIS tank in order to create a very well defined fission neutron source.

The Iron88 benchmark experimental array, which was assembled in the ASPIS tank, was comprised of three regions: the source region with the fission plate, 13 mild steel plates each roughly 5.1 cm thick and a mild- stainless-steel backing shield. Void gaps were left between the mild steel plates for the various (Sulphur, Indium, Rhodium, Gold, Aluminium) activation foil detectors.

The models developed in the scope of this report were developed from scratch, they are not based on any other models available for other transport codes or other, simplified, models for MCNP. However the source distribution is based but modified on a MCNP model produced by Alberto Milocco. In the first step CAD models (2.1) were produced for each of the activation foil detectors reported in the SINBAD documentation. The CAD models were used as the base for MCNP geometrical modelling (2.2). The material (2.2.1), source (2.2.2) and tally (2.2.3) modelling was based on the SINBAD documentation. Finally optimal variance reduction parameters were produced after several iteration of the ADVANTG input parameters (3).

2.1 CAD modelling

CAD model were developed with the Rhinoceros 5 (Rhino) software [12]. The CAD models can be used in further neutron transport analysis with other transport codes. The CAD models also contain all of the dimensions crucial for development of other models. They are also extremely useful for visualization purposes.

The dimension for the CAD models were mainly taken form the SINBAD documentation, specifically the two following reports:

- G.A. Wright, M. J. Grimstone, Benchmark Testing of JEF-2.2 Data for Shielding Applications: Analysis of the Winfrith Iron 88 Benchmark Experiment, Report No. AEA-RS-1231, EFF-Doc-229 and JEF-Doc-421 (1993).

- G. A. Wright, A. Avery, M. J. Grimstone, H. F. Locke, S. Newbon, Benchmarking of the JEFF2.2 Data Library for Shielding Applications, Proceedings, 8th International Conference on Radiation Shielding, April 24-28, 1994, Arlington, Texas, U.S.A., vol.2, p.816.

Both of the reports mentioned are available in the SINBAD database.

A sample CAD model of the Aluminium activation foil detector case with the major dimensions is presented in Figures 2.1 and 2.2. The CAD models are available from the author on demand.

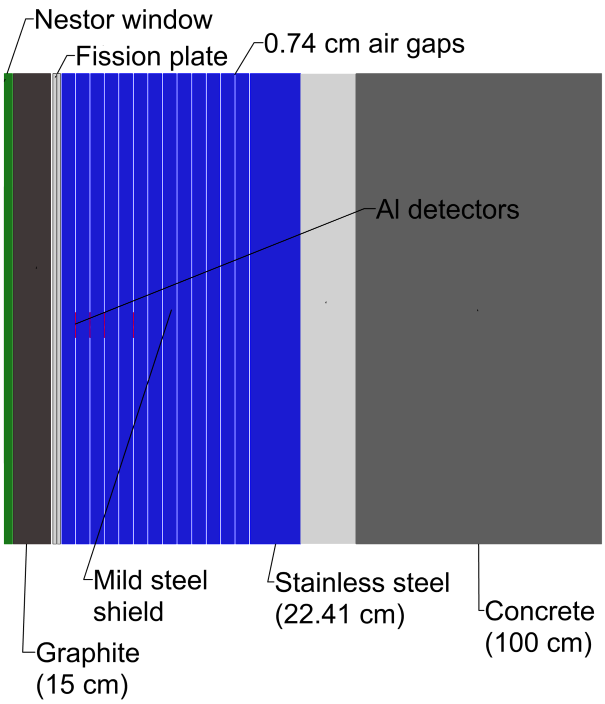

Figure 2.1: CAD model of the ASPIS Iron88 SINBAD benchmark experiment - Aluminium detectors. All dimensions are in centimeters.

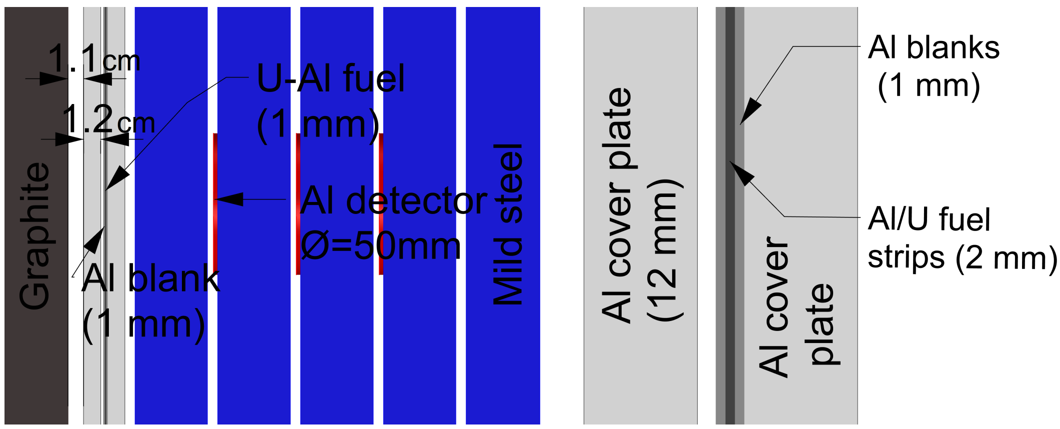

Figure 2.2: CAD model of the ASPIS Iron88 SINBAD benchmark experiment - Aluminium detectors. Details of the Aluminium detectors (left) and of the fission plate (right). Dimensions are in centimeters and millimeters.

2.2 MCNP modelling

The geometrical modelling in MCNP was done using the GRASP [13] CAD to MCNP conversion tool developed at JSI ("Jožef Stefan" Institute) by the author of the report. The MCNP models dimension correspond directly to those in the CAD models. Geometrical modelling based on pre-developed CAD models has proven to be straight forward and fast.

Selected MCNP models which correspond to the CAD models shown in Figures 2.1 and 2.2 are presented as Figures 2.3 and 2.4. The MCNP models where visualized with the MCNP Visual Editor [14]. The different colours correspond to different materials used in the model. The definition of material is described in the next section of the report (2.2.1). The geometrical characteristics are converted from CAD format in-to MCNP format without any loss of detail using the GRASP tool.

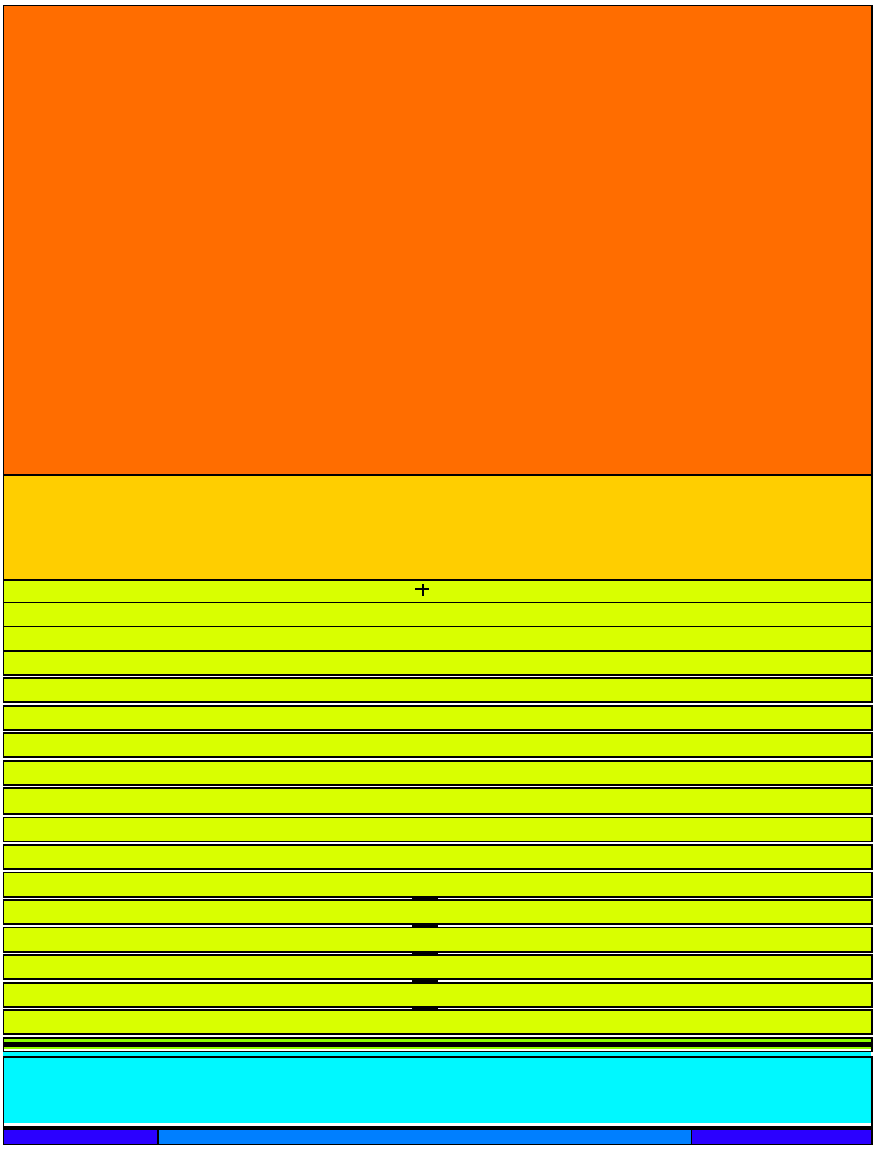

Figure 2.3: MCNP model X-Y cross section of the ASPIS Iron88 SINBAD benchmark experiment - Aluminium detectors. All dimensions are in centimeters.

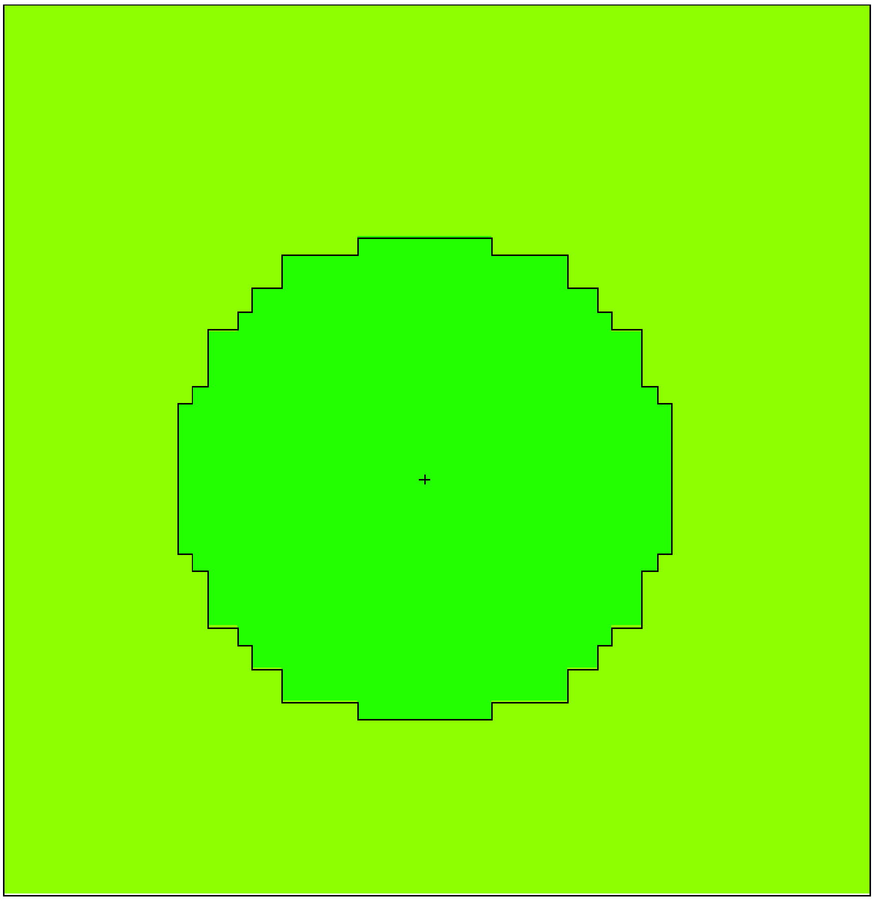

Figure 2.4: MCNP model X-Z cross section of the ASPIS Iron88 SINBAD benchmark experiment - Aluminium detectors.

2.2.1 Materials

The materials for the MCNP input files were defined based on the information in the SINBAD documentation (as88-exp.htm Table 2). 8 main materials (designated with *Material Ref. No.* in the original SINBAD documentation) were defined alongside the various activation materials and dummy materials used for reaction rate calculations.

The materials in the SINBAD documentation are given per element, but for MCNP calculations per nuclide definitions of the materials were needed. The MATSSF code [15] was used to calculate the per nuclide atomic densities.

Materials for the activation foil detectors were also defined based on the SINBAD documentation, namely Paragraph *4. Measurement System and Uncertainties* in file as88-abs.htm. The exact material definitions and densities used can be found in the appended MCNP input file in Appendix B.

2.2.2 Source

The source was modelled as a fixed source (SDEF keyword in MCNP) with a spatial distribution that corresponds to the information given in the SINBAD documentation. The source spatial distribution was modelled with th "A" option with the SI (source information) auxiliary cards - meaning the source probabilities are given at exactly SI positions, and the probabilities between two SI entries are linearly interpolated. The SI entries were defined in such a way to preserve the integral per-bin probability given in *Table 3: Source distribution on the fission plate* from the SINBAD documentation (as88-exp.htm file). The source spatial distribution is based on previous work done by A. Milocco [16].

The energy spectra of the source is not specifically given in the SINBAD or original documentation. The source energy spectra is only said to be a *"fission energy spectrum of the source is that of neutrons emitted from the fission of U-235" (as88-abs.htm, 3. Description of the Source and Experimental Configuration).* Considering this the Watt spectrum and IAEA Standards-2017 Prompt fission neutron spectra (PFNS) from thermal neutrons induced on ^{235}U were used [17].[1] The IAEA PFNS spectrum is available at: https://www-nds.iaea.org/standards/ref-spectra/PFNS-u235nth.txt. A per-bin definition of the source energy spectra was chosen for better compatibility with ADVANTG's source biasing capabilities. A separate sensitivity study to the source energy spectra was performed [4], but the information on the source energy/spatial distribution need to be studied further and analysed.

2.2.3 Detectors/tallies

Each detector was modelled as a F4 volume tally with the actual detector modelled as a cylinder with the appropriate height and diameter. The dimensions of each detector are given in the original SINBAD documentation (as88-abs.htm file) under Section *4. Measurement System and Uncertainties.* The F4 tally was modified using the FM card to produce appropriate reaction rates. The cross sections for the reaction rates (Al, S, Rh, In) from the International Reactor Dosimetry and Fusion File IRDFF v.1.05 [11] are shown in Figure 2.5. The cylinder was filled with the corresponding detector material.

[1] An alternative version of the inputs exists with a Watt fission spectra source. The source is defined in 640 energy groups using an auxiliary ADVANTG [10] utility (watt.py). Comparison of the results with the Watt source spectra and the 2017 IAEA prompt fission neutron spectra is given in Appendix A. The inputs are available from the author.

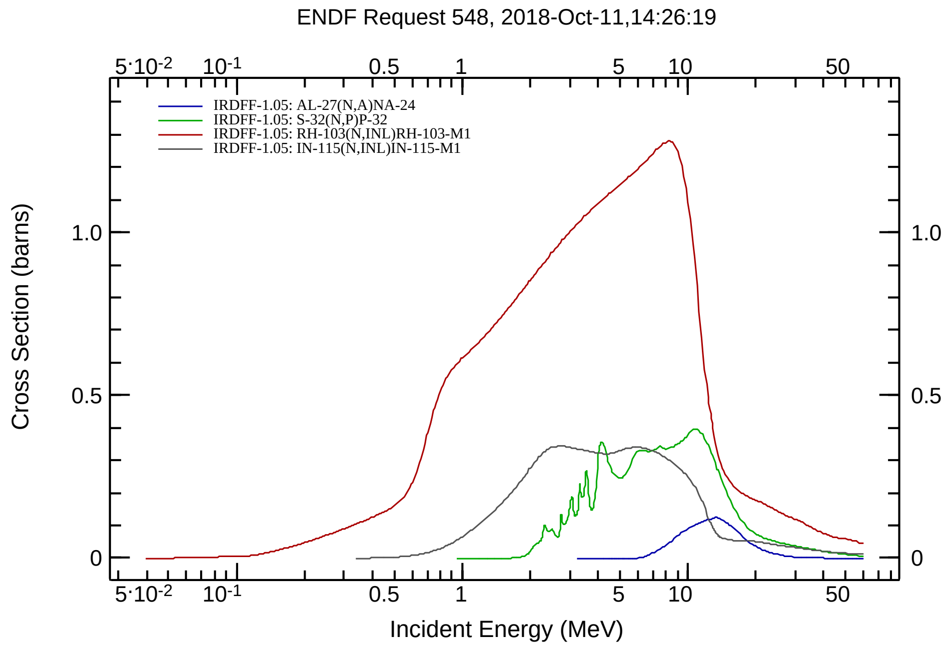

Figure 2.5: Dosimetry reaction cross sections used for reaction rate calculations using the FM card from the International Reactor Dosimetry and Fusion File IRDFF v.1.05.

For absolute comparison to the experimental results, such as the ones in the Results section 5 of the report, the tally results (RR_{MCNP}) are normalized according to the SINBAD documentation (as88-exp.htm file) in the Section named *Source description*. The normalization factor is calculated with the following equation 2.1:

$$\begin{aligned} RR_{normalized} &= RR_{MCNP} * NP * FP * \bar{\nu} * FpW/b \\ &= RR_{MCNP} * 1.296 \cdot 10^{-12} \end{aligned} \quad (2.1)$$

Where the factors in equation 2.1 are:

- RR_{MCNP} = F4 MCNP tally modified using the FM card and the appropriate cross-section
- NP = NESTOR power = 30 kW
- FP = fission plate power normalized to NESTOR power = $5.68 \cdot 10^{-4}$ W/W$_{\text{NESTOR}}$ (Watts-per-NESTOR-Watt)
- $\bar{\nu}$ = average number of neutrons per fission = 2.437

- FpW = average number of fissions per Watt = $3.121 \cdot 10^{10}$
- b = barn = 10^{24} cm

3 Variance reduction

Because this is a deep shielding problem variance reduction was needed to perform effective and fast simulations. The variance reduction was performed by limiting the physical properties of the transport problem and generation of energy and space dependent weight windows alongside a spatially and energy biased source by the ADVANTG hybrid deterministic/Monte Carlo code.

The physical parameters of the problem were limited using the *cut* card to stop the neutron transport at a certain energy threshold. The energy threshold was determined based on the detectors specific reaction cross sections from the IRDFF libray [11].

The final step was to produce energy and space dependent weight windows and source biasing parameters with ADVANTG. The procedure is described in the following Section (3.1).

3.1 ADVANTG

The **A**utomate**D** **VA**ria**N**ce reduc**T**ion [10] (ADVANTG) hybrid deterministic/Monte Carlo transport code developed at ORNL was used to determine energy and space dependent weight window (WW) variance reduction parameters and source biasing parameters. The source energy spectra was also produced by a utility included in ADVANTG based on the Watt fission spectra.

The Forward-Weighted Consistent Adjoint Driven Importance Sampling [18] (FW-CADIS) method was used to determine the WW windows for multiple detector (tally) locations. FWCADIS response weighting was turned on. The bplus multigroup nuclear data library included with the ADVANTG distribution was used for all cases for the initial deterministic calculation. A simple symmetric quadrature set was defined along with a high order (P_n=5) of expansion of the scattering angle. A detailed Cartesian mesh used for the deterministic calculation was defined for each case, taking in to account the mean free paths of neutron at appropriate energies for each shielding material.

When we compare the Figure-of-merit (FOM) statistical test of the analog[2] MCNP calculation to a ADVANTG accelerated MCNP calculation for the case of the Sulphur detector, the speed-up factor or relative FOM ($FOM_{rel} = \frac{FOM_{ADVANTG}}{FOM_{analog}}$) for the closest detector locations (A2) is about 4 but it increases for the farthest positions. For position A15 the speed-up factor of the simulation is about $3 \cdot 10^5$. A comparison of a long analog MCNP calculation with 10^{10} neutron particle histories simulated to an ADVANTG accelerated calculation, with 10^7 neutron particle histories is shown in

[2] A MCNP calculation where WW were not used.

3.1. The $C_{ADVANTG}/C_{Analog}$ value is 1 within the combined 1σ statistical uncertainty for locations A2 - A10 which shows no bias is introduced in to the calculation with ADVANTG produced variance reduction parameters. The statistical uncertainty of the analog simulations for locations A11 - A15 becomes so large that the simulation results become questionable, hence the C/C values have little meaning. Nonetheless the ADVANTG accelerated calculations for these locations still have a relative uncertainty under 2 %.

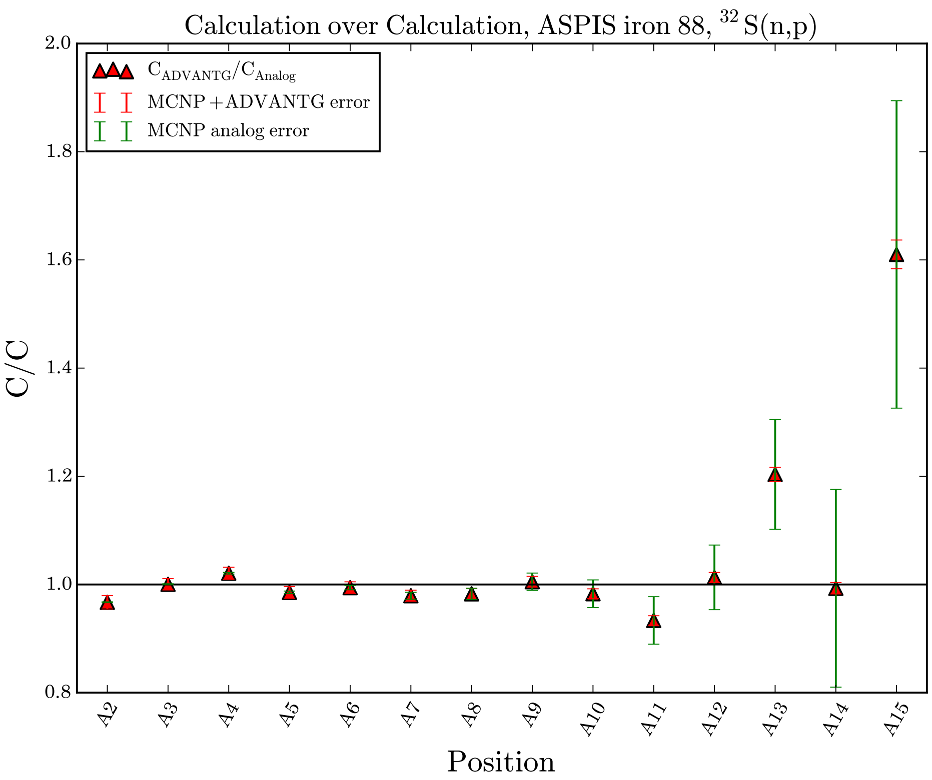

Figure 3.1: $C_{ADVANTG}/C_{Analog}$ (Calculation-over-calculation) comparison of ADVANTG accelerated MCNP calculation to an analog MCNP calculation of the Sulphur detector.

Using all of the above mentioned variance reduction parameters statistical uncertainties bellow 2 % (in most cases bellow 1 %) for Sulphur, Indium, Rhodium and Aluminium detector materials and locations are achieved in under 5 min on a local computer cluster with 40 threads (Intel Xeon E5-2680 v2).

ADVANTG was also used to speed-up the Gold activation foil cases, but the preliminary calculations given in this report are analog MCNP calculation to eliminate the possibility of introducing additional uncertainties in to the preliminary results. More on this in Sections 4, 5 and 5.4.

It should be noted that all of the simulations were done using MCNP5. version 1.6. ADVANTG was designed using this version of MCNP. The produced WW are compatible with MCNP6, but in some cases MCNP6 is slower. It has also been reported that in some cases MCNP6 reports failed statistical tests on the tallies where MCNP5 ver. 1.6 does not. But the mean values between the two releases doesn't differ. All of the WW produced in the scope of this work were also testes with MCNP6 and no significant difference between the mean results of the two MCNP releases was noted.

4 Open issues in the modelling

The models produced are a complete set of MCNP input files and effective variance reduction parameters of the APSIS Iron88 benchmark experiments. In the case of deep shielding problems and fission spectra source neutrons effective variance reduction parameters are crucial for nuclear data validation and evaluation processes - especially for nuclear data adjustment efforts, where several simulations are needed for a successful analysis. Despite the completeness and quality of the models some issues remain open which will have to be addressed in further evaluations. The following issues remain:

- Source energy spectra - the source energy spectra is only reported as being: *"fission energy spectrum of the source is that of neutrons emitted from the fission of U-235" (as88-abs.htm, 3. Description of the Source and Experimental Configuration).* A sensitivity to the different fission energy spectra was performed [4], but reliable information on the uncertainties in PFNS and spatial distribution are needed.

- Source spatial distribution - the spatial distribution of the fission source in the fission plate is described in detail. A sensitivity study was performed in order to ascertain the effect of the distribution on the calculated reaction rates. The spatial distribution has impact on the calculated reaction-rates close to the fission plate, but the uncertainty in spatial distributions was not reported.

- Block of graphite in front of the fission plate - in the case of the Gold activation detectors the thermal neutrons originating directly from the NESTOR reactor can significantly affect the experimental results. In order to approximately reproduce this effect with the simulation models, an addition of a block of graphite located before the fission plate was proposed by the experimental evaluators ([1], section 3.1 Geometry modelling). An improvement of the C/E results closest (A2-A4) to the fission plate were observed. However, addition of the graphite block also effects the gold reaction rates further away from the source, by as much as $\sim 10\%$. Additional sensitivity studies are needed to ascertain the uncertainties linked with adding a block of graphite.

- Results for Gold are only preliminary - at this stage the Gold activation results are not suitable for data validation applications. Additional studies to determine the impact of the additional graphite block positioned in front of the fission plate, mentioned in the previous bullet, are needed. Furthermore, a sensitivity study of the source energy spectra is needed alongside a study to determine the effect of thermal neutrons which originate directly from the NESTOR reactor.

5 Results

Results simulated using MCNP5 ver 1.6 with the ENDF/B-VII.1, ENDF/B-VIII, JEFF-3.3 and JENDL-4.0u nuclear data libraries are given in this Section. Whichever nuclear data library of the four was used, the cross-section for the reaction rate calculation was always taken from the International Reactor Dosimetry and Fusion File IRDFF v.1.05 [11]. The results for five different activation foil detectors are presented, Sulphur 5.1, Indium 5.2, Rhodium 5.3, Gold 5.4 and Aluminium 5.5. Some comments on each of the activation foil C/E (Calculation over Experiment) results are given in the following sub-sections.

5.1 Sulphur - $^{32}S(n,p)$

Arguably the most interesting are the sulphur results. The ENDF/B-VII.1 and JENDL-4.0u C/E results agree reasonably well even for the farthest locations, where the ENDF/B-VII.1 performs slightly better with a small under-prediction of the experimental results. On the other hand the newest nuclear data libraries ENDF/B-VIII and JEFF-3.3 give completely opposite results for the farthest locations, where ENDF/B-VIII under-predicts and JEFF-3.3 over-predicts the experimental results.

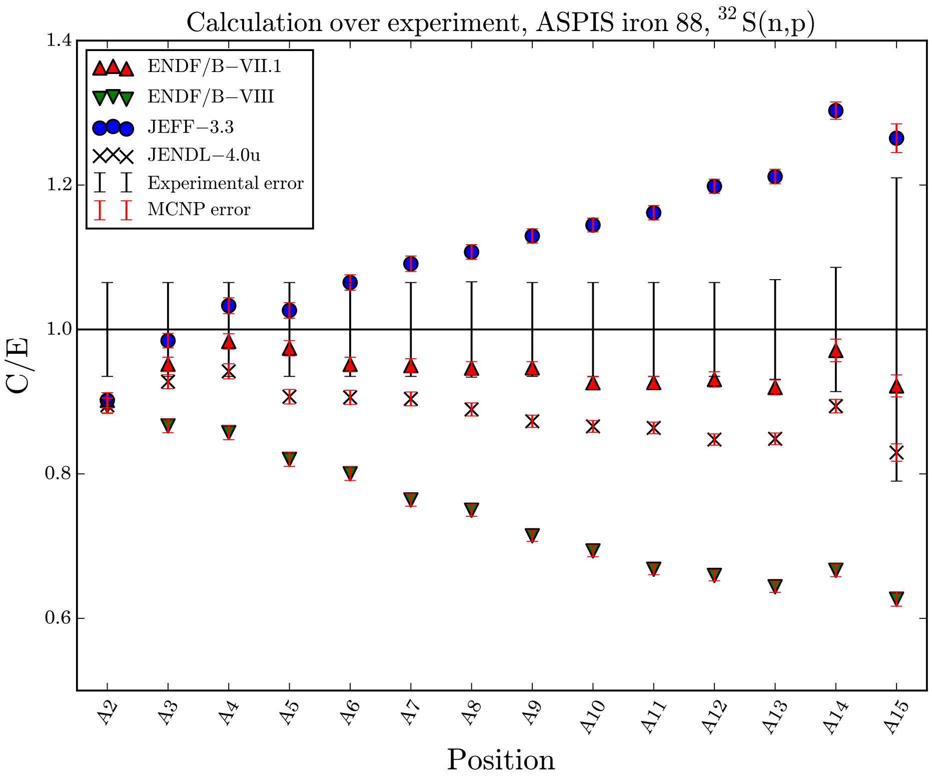

Figure 5.1: C/E (Calculation over Experiment) results for Sulphur detectors at increasingly distant locations (A2 - A15).

5.2 Indium - ^{115}In(n,n')

An interesting trend is also seen in the indium foil activation results where the JEFF-3.3 nuclear data library performs the best with only a small over-prediction of the results for all experimental position. For the three other nuclear data libraries (ENDF/B-VII.1, ENDF/B-VIII and JENDL-4.0u) an increasing under-prediction of the results is observed, where ENDF/B-VIII performs the worst.

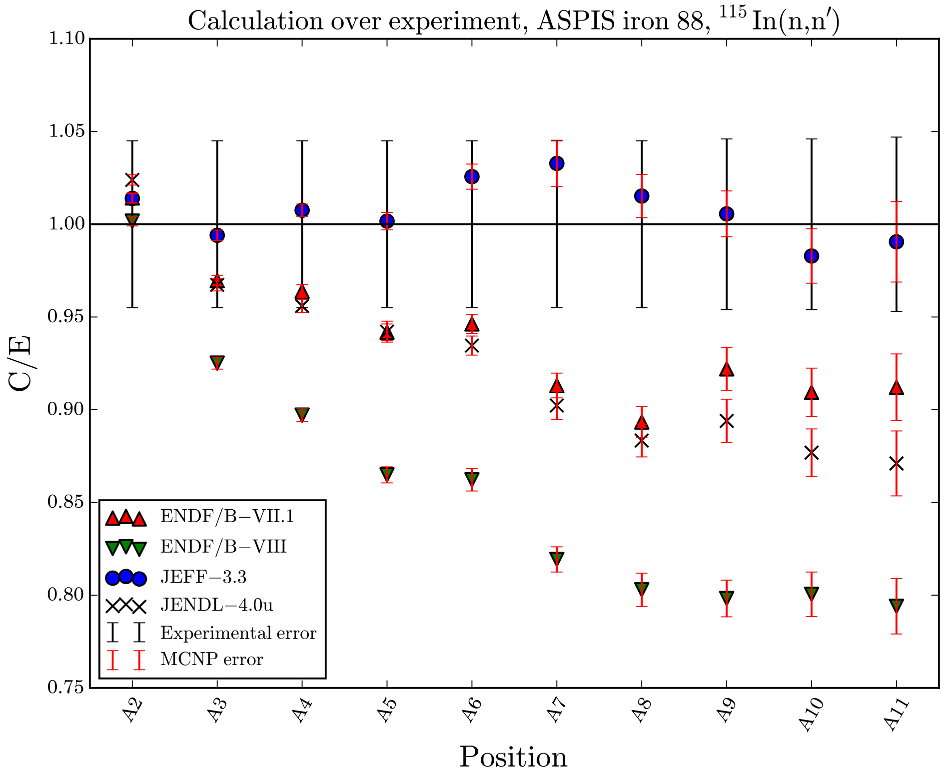

Figure 5.2: C/E (Calculation over Experiment) results for Indium detectors at increasingly distant locations (A2 - A11).

5.3 Rhodium - ^{103}Rh(n,n')

In case of the rhodium foil activation results all of the libraries (ENDF/B-VII.1, ENDF/B-VIII, JEFF-3.3 and JENDL-4.0u) perform almost equally with a slight over-prediction of the results throughout.

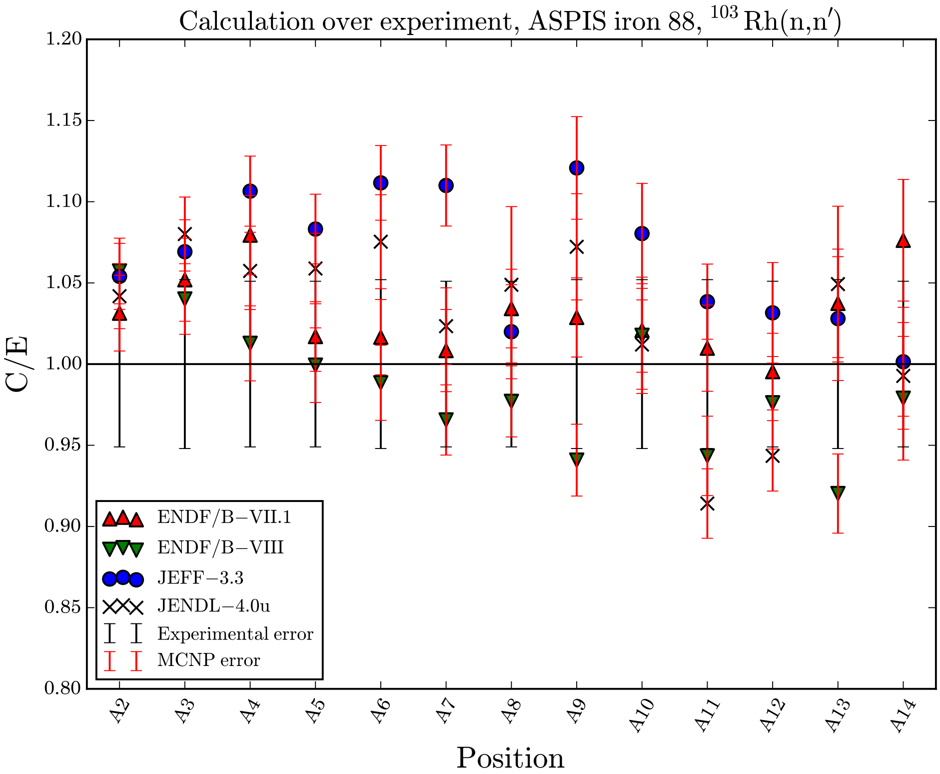

Figure 5.3: C/E (Calculation over Experiment) results for Rhodium detectors at increasingly distant locations (A2 - A14).

5.4 Gold - ^{197}Au(n,γ) preliminary results

The results given in this report for Gold are only preliminary. Especially the results for locations closer to the fission plate (A2 - A5) are highly dependent on the thermal neutrons which originated directly from the NESTOR reactor. With the available benchmark information it is currently not possible to accurately model this effect.

At this stage these Gold results and model are not recommended for nuclear data validation. Results for locations farther away from the fission plate, and consequently the NESTOR reactor, are more reliable and could be used for nuclear data validation after an additional sensitivity study which shall permit to determine realistic uncertainties to be assigned to these values. ADVANTG was not used to speed-up these calculations to eliminate the possibility of introducing additional uncertainties in to the results.

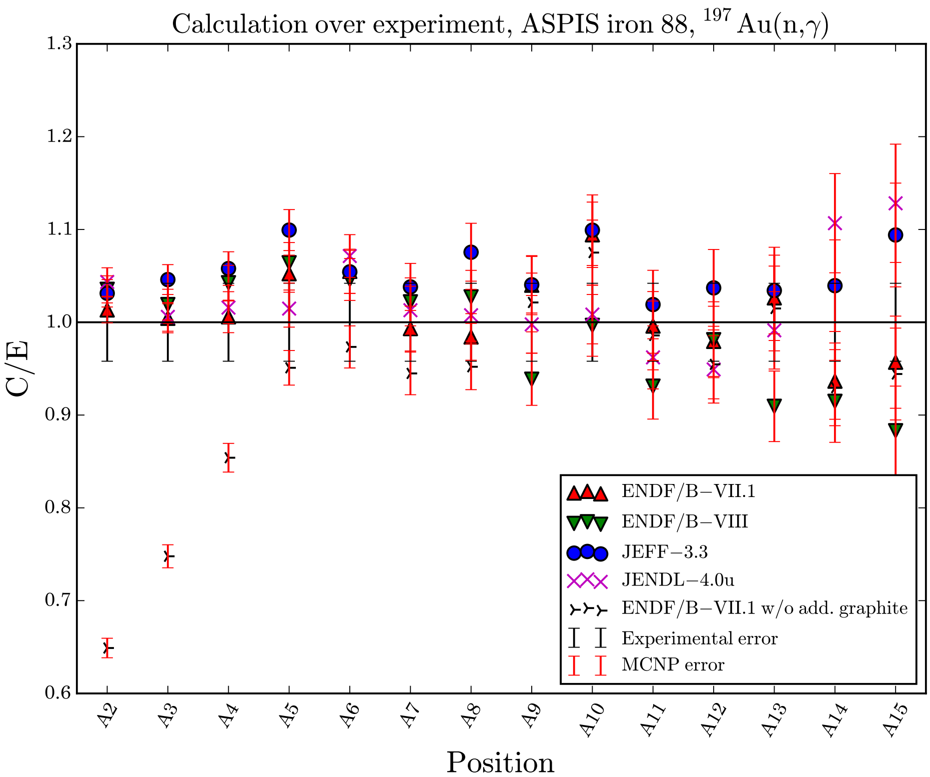

Figure 5.4: Preliminary C/E (Calculation over Experiment) results for Gold detectors at increasingly distant locations (A2 - A15).

5.5 Aluminium - ^{27}Al(n,α)

The results for the aluminium foil activation detectors show an over-prediction for all experimental positions and the four nuclear data libraries. Among the four tested libraries, the ENDF/B-VIII library performs the best, where the C/E results are around 1.1.

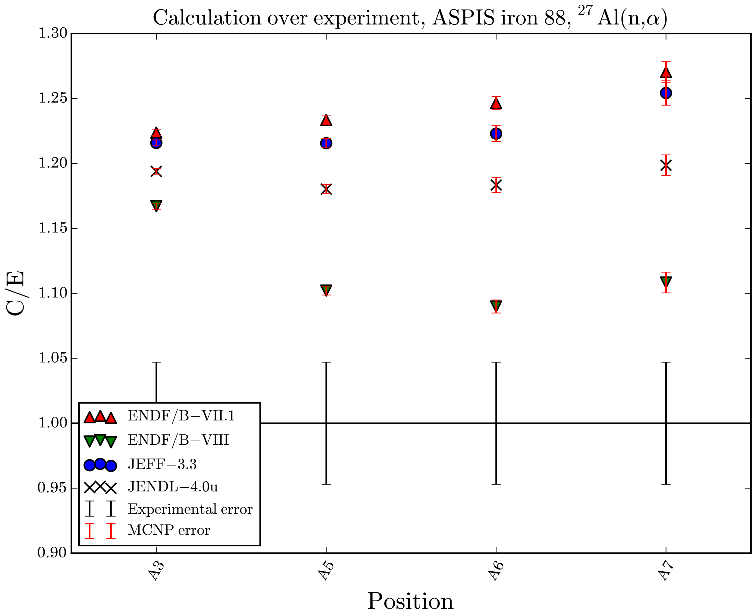

Figure 5.5: C/E (Calculation over Experiment) results for Aluminium detectors at increasingly distant locations (A3, A5, A6, A7).

6 Conclusion

The models produced are a complete set of MCNP input files and effective variance reduction parameters of the APSIS Iron88 benchmark experiments. In the case of deep shielding problems and fission spectra source neutrons effective variance reduction parameters are crucial for nuclear data validation and evaluation processes - especially for nuclear data adjustment efforts, where several simulations are needed for a successful analysis.

The models were developed starting with CAD models based on original documentation gathered in the SINBAD database distribution. CAD models for all five different activation foil material detectors were produced. Based on CAD models the MCNP geometrical models were produced. The material, source and tally (detector) information was taken form the SINBAD documentation.

Variance reduction was implemented including simulation energy cut off's, energy and spatial source biasing parameters and space and energy dependent weight windows. Weight window variance reduction parameters were produced for all cases in order to speed-up the convergence of all detectors/tallies in a single simulation. A speed-up of the farthest detector locations (A15) of the sulphur activation foil detectors was about $3{\cdot}10^5$, and no bias was introduced to the calculation.

Results simulated using MCNP5 ver 1.6 with the ENDF/B-VII.1, ENDF/B-VIII, JEFF-3.3 and JENDL-4.0u nuclear data libraries were presented. The results for five different activation foil detectors Sulphur, Indium, Rhodium, Gold and Aluminium were given. A large difference between different nuclear data libraries was observed when analysing the Indium, Aluminium and especially Sulphur activation foil results. A large discrepancy between the the newest nuclear data libraries JEFF-3.3 and ENDF/B-VIII for the Sulphur case was observed. The results for Rhodium do not differ by much for the different nuclear data libraries. The results for the Gold activation foils are only preliminary at this point and are not recommended for nuclear data validation purposes. An additional sensitivity study for the gold activation foils is needed.

References

[1] G.A. Wright and M. J. Grimstone. *Benchmark Testing of JEF-2.2 Data for Shielding Applications: Analysis of the Winfrith Iron 88 Benchmark Experiment.* Report No. AEA-RS-1231, EFF-Doc-229 and JEF-Doc-421. 1993.

[2] I. Kodeli and A. F. Avery. *Winfrith Iron 88 Benchmark (ASPIS).* SINBAD compilation NEA-1517/35.

[3] I. Kodeli and L. Plevnik. “Nuclear data adjustment exercise combining information from shielding, critical and kinetics benchmark experiments ASPIS-Iron 88, Popsy and SNEAK-7A/7B”. In: 106 (Apr. 2018).

[4] I. Kodeli. “Transport and S/U analysis of the ASPIS-IRON88 Benchmark using recent and older iron cross-section evaluations”. In: *PHYSOR 2018: Reactor physics paving the way towards more efficient systems.* American Nuclear Society, Inc. 2018.

[5] I. Kodeli et al. “20 Years of SINBAD (Shielding Integral Benchmark Archive and Database)”. In: *Progress in Nuclear Science and Technology* 4 (2014), pp. 308–311.

[6] I. Kodeli. “Introduction to SINBAD - tutorial”. In: *RPSD-2018: 20th Topical meeting of the radiation protection and shielding division.* American Nuclear Society, Inc. 2018.

[7] I. Kodeli. “Nuclear Data and Code Testing Using the Radiation Shielding Experiments in SINBAD”. In: *M& C 2017: International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering.* On USB. 2017.

[8] I. Kodeli, G. Žerovnik, and A. Milocco. “Examples of Recent Use of SINBAD Database for Nuclear Data and Code Validation”. In: *ICRS-13 & RPSD-2016 Conference.* 2016.

[9] X-5 Monte Carlo Team. *MCNP — A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory.* LA-UR-03-1987. 2003.

[10] S.W. Mosher. *ADVANTG-An Automated Variance Reduction Parameter Generator.* ORNL/TM-2013/416 Rev. 1, Oak Ridge National laboratory. 2015.

[11] R. Capote et al. *Summary Description of the New International Reactor Dosimetry and Fusion File (IRDFF release 1.0).* J. ASTM International, Volume 9, Issue 4, April 2012, JAI104119, Technical report INDC(NDS)-0616, IAEA, Vienna. 2012.

[12] Robert McNeel & Associates. *Rhinoceros 5 User’s Guide For Windows*. 2004.

[13] B. Kos and L. Snoj. “On using grasshopper add-on for CAD to MCNP conversion”. In: *PHYSOR 2016: Unifying Theory and Experiments in the 21st Century.* American Nuclear Society, Inc. 2016.

[14] A.L. Schwarz, R.A. Schwarz, and L.L. Carter. *MCNP/MCNPX Visual Editor Computer Code Manual*. 2008.

[15] A. Trkov et al. “On the Self-Shielding Factors in Neutron Analysis”. In: *Nuclear Instruments and Methods in Physics Research* A.610 (2009), pp. 553–565.

[16] A. Milocco. *Quality Assessment of SINBAD Evaluated Experiments ASPIS Iron (NEA-1517/34), ASPIS Iron-88 (NEA-1517/35), ASPIS Graphite (NEA-1517/36), ASPIS Water (NEA-1517/37), ASPIS N/G Water/Steel (NEA-1517/49), ASPIS PCA Replica (NEA-1517/75)*. 2015.

[17] A. Trkov and R. Capote. “Evaluation of the Prompt Fission Neutron Spectrum of Thermal-neutron Induced Fission in U-235”. In: *Physics Procedia* 64 (2015). Scientific Workshop on Nuclear Fission Dynamics and the Emission of Prompt Neutrons and Gamma Rays, THEORY-3, pp. 48–54.

[18] J. C. Wagner and S. W. Mosher. *Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Reactor Analyses*. 2010.

A Comparison of results with the IAEA 2017 standard and Watt prompt fission neutron source spectra

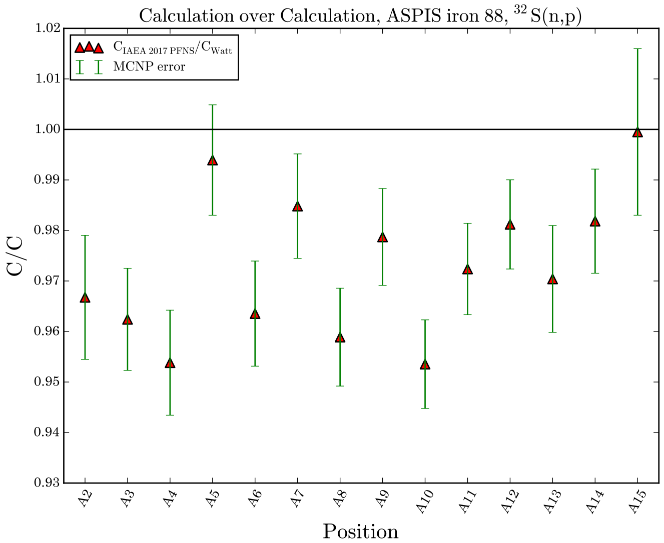

Figure A.1: C/C (Calculation over Calculation) results for Sulphur detectors at increasingly distant locations with the Watt and the 2017 IAEA standard prompt fission neutron source spectra.

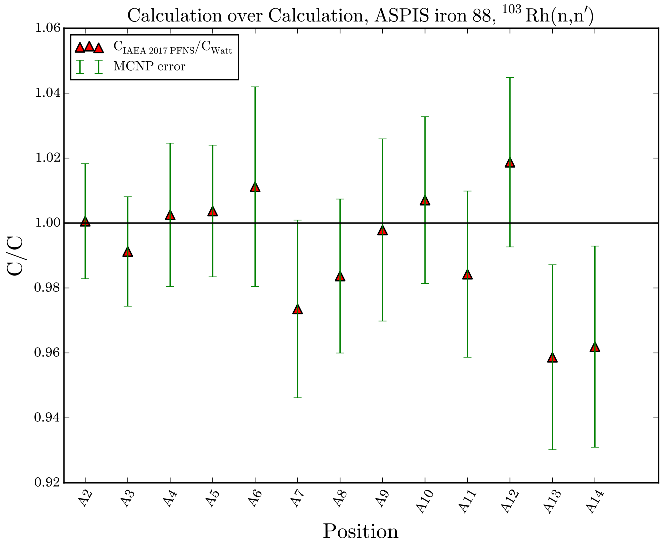

Figure A.2: C/C (Calculation over Calculation) results for Rhodium detectors at increasingly distant locations with the Watt and the 2017 IAEA standard prompt fission neutron source spectra.

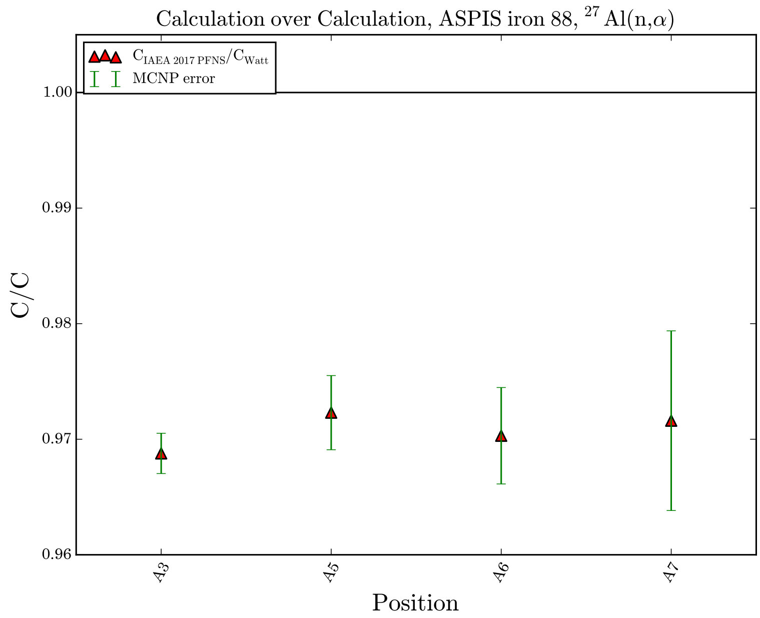

Figure A.3: C/C (Calculation over Calculation) results for Aluminium detectors at increasingly distant locations with the Watt and the 2017 IAEA standard prompt fission neutron source spectra.

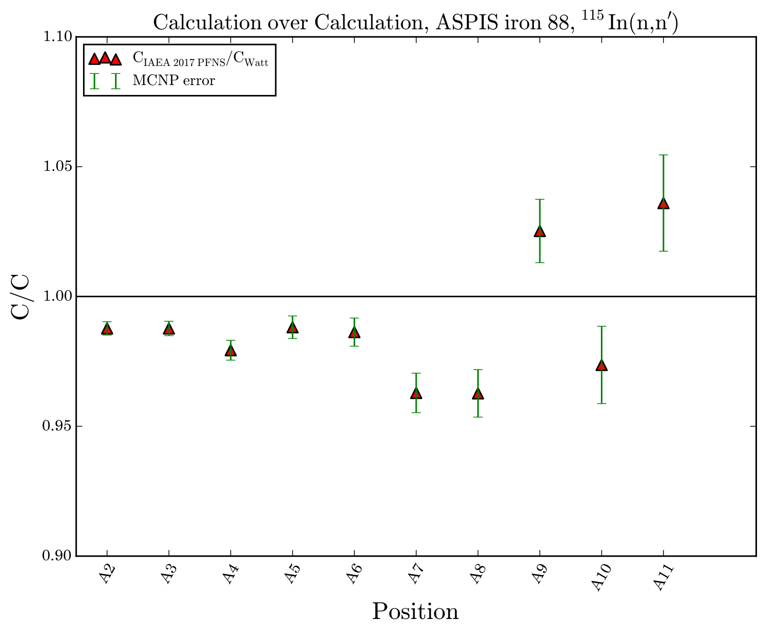

Figure A.4: C/C (Calculation over Calculation) results for Indium detectors at increasingly distant locations with the Watt and the 2017 IAEA standard prompt fission neutron source spectra.

B Sample ASPIS iron MCNP input

```
ASPIS iron 88 Al - Aluminium, B. Kos (bor.kos@ijs.si), 2018
c Based on SINBAD documentation (iron_88.pdf Benchmark testing of JEF2.2 data
c for shielding applications: Analysis of the Winfrith iron 88 benchmark experiment)
c Source distributon based, but moddified, on MCNP input file by Alberto Milocco,
c Alberto.Milocco@mib.infn.it
c Bor Kos, JSI, August 2018
c -------------------------------------------------------------------------------
c         CELLS
c -------------------------------------------------------------------------------
c Shields
c
1  6 0.0853705  -300 imp:n=1
2  6 0.0853705  -301 imp:n=1
3  6 0.0853705  -302 imp:n=1
4  6 0.0853705  -303 imp:n=1
5  6 0.0853705  -304 imp:n=1
6  6 0.0853705  -305 imp:n=1
7  6 0.0853705  -306 imp:n=1
8  6 0.0853705  -307 imp:n=1
9  6 0.0853705  -308 imp:n=1
10 6 0.0853705  -309 imp:n=1
11 6 0.0853705  -310 imp:n=1
12 6 0.0853705  -311 imp:n=1
13 6 0.0853705  -312 imp:n=1
14 6 0.0853705  -313 imp:n=1
15 6 0.0853705  -314 imp:n=1
16 6 0.0853705  -315 imp:n=1
17 6 0.0853705  -316 imp:n=1
18 7 0.0864102  -317 imp:n=1
19 8 0.0793442  -318 imp:n=1
c Aluminium NESTOR reactor window
20 1 0.0852154  -209 210 imp:n=1
21 2 0.060261   -210     imp:n=1
c  Graphite block
22 3 0.082729  -211 imp:n=1
c  Aluminium before and after fission plate
23 5 0.0593267 -212 imp:n=1
24 5 0.0593267 -213 imp:n=1
c Fission plate
```

```
25 4 0.0597907 -201:-202:-203:-204:-205:-206:-207 imp:n=1
c Aluminium arround fission plate
26 5 0.0593267 -208 #25 imp:n=1
c Detectors
c A3
101 101 0.061308 -401 imp:n=1
c A4
102 101 0.061308 -402 imp:n=1
c A5
103 101 0.061308 -403 imp:n=1
c A6
104 101 0.061308 -404 imp:n=1
c A7
105 101 0.061308 -405 imp:n=1
c Void and rest of the world
200 0 -1 #1 #2 #3 #4 #5 #6 #7 #8 #9 #10 #11 #12 #13 #14 #15 #16 #17 #18 #19
#20 #21 #22 #23 #24 #25 #26
#101 #102 #103 #104 #105
imp:n=1
201 0  1 imp:n=0

c -------------------------------------------------------------------------------
c         SURFACES
c -------------------------------------------------------------------------------
c Void and rest of the world
1 sy 75 200
c Fission plate
201 box -52.25 -0.05 -15.88 0.0 0.0 31.76  0.0 0.2 0.0 104.5 0.0 0.0
202 box -49.08 -0.05 -19.69 0.0 0.0 39.38  0.0 0.2 0.0 98.16 0.0 0.0
203 box -45.92 -0.05 -31.75 0.0 0.0 63.5   0.0 0.2 0.0 91.84 0.0 0.0
204 box -39.58 -0.05 -35.56 0.0 0.0 71.12  0.0 0.2 0.0 79.16 0.0 0.0
205 box -36.42 -0.05 -40.64 0.0 0.0 81.28  0.0 0.2 0.0 72.84 0.0 0.0
206 box -30.08 -0.05 -47.63 0.0 0.0 95.26  0.0 0.2 0.0 60.16 0.0 0.0
207 box -14.25 -0.05 -51.44 0.0 0.0 102.88 0.0 0.2 0.0  28.5 0.0 0.0
c Aluminium arround fission plate
208 box -88.9  -0.15 -88.9 0.0 0.4   0.0 182.9 0.0 0.0 0.0 0.0 190.0
c Aluminium NESTOR reactor window
209 box -88.9  -21.25 -88.9 0.0 3.18 0.0 182.9 0.0 0.0 0.0 0.0 190.0
210 rcc 0.0 -21.25 0.0 0.0 3.18 0.0 56.06
c Graphite block
211 box -88.9  -17.55 -88.9 0.0 15.0 0.0 182.9 0.0 0.0 0.0 0.0 190.0
```

```
c Aluminium before and after fission plate
212 box -88.9  -1.45 -88.9 0.0 1.2 0.0 182.9 0.0 0.0 0.0 0.0 190.0
213 box -88.9   0.25 -88.9 0.0 1.2 0.0 182.9 0.0 0.0 0.0 0.0 190.0
c Shields
300 box -88.9  2.19  -88.9 0.0 5.10  0.0 182.9 0.0 0.0 0.0 0.0 190.0
301 box -88.9  8.03  -88.9 0.0 5.12  0.0 182.9 0.0 0.0 0.0 0.0 190.0
302 box -88.9 13.89  -88.9 0.0 5.12  0.0 182.9 0.0 0.0 0.0 0.0 190.0
303 box -88.9 19.75  -88.9 0.0 5.10  0.0 182.9 0.0 0.0 0.0 0.0 190.0
304 box -88.9 25.59  -88.9 0.0 5.20  0.0 182.9 0.0 0.0 0.0 0.0 190.0
305 box -88.9 31.53  -88.9 0.0 5.15  0.0 182.9 0.0 0.0 0.0 0.0 190.0
306 box -88.9 37.42  -88.9 0.0 5.20  0.0 182.9 0.0 0.0 0.0 0.0 190.0
307 box -88.9 43.36  -88.9 0.0 5.20  0.0 182.9 0.0 0.0 0.0 0.0 190.0
308 box -88.9 49.30  -88.9 0.0 5.25  0.0 182.9 0.0 0.0 0.0 0.0 190.0
309 box -88.9 55.29  -88.9 0.0 5.18  0.0 182.9 0.0 0.0 0.0 0.0 190.0
310 box -88.9 61.21  -88.9 0.0 5.07  0.0 182.9 0.0 0.0 0.0 0.0 190.0
311 box -88.9 67.02  -88.9 0.0 5.12  0.0 182.9 0.0 0.0 0.0 0.0 190.0
312 box -88.9 72.88  -88.9 0.0 5.18  0.0 182.9 0.0 0.0 0.0 0.0 190.0
313 box -88.9 78.80  -88.9 0.0 5.10  0.0 182.9 0.0 0.0 0.0 0.0 190.0
314 box -88.9 83.90  -88.9 0.0 5.25  0.0 182.9 0.0 0.0 0.0 0.0 190.0
315 box -88.9 89.15  -88.9 0.0 5.00  0.0 182.9 0.0 0.0 0.0 0.0 190.0
316 box -88.9 94.15  -88.9 0.0 4.97  0.0 182.9 0.0 0.0 0.0 0.0 190.0
317 box -88.9 99.12  -88.9 0.0 22.41 0.0 182.9 0.0 0.0 0.0 0.0 190.0
318 box -88.9 121.53 -88.9 0.0 100.0 0.0 182.9 0.0 0.0 0.0 0.0 190.0
c Detectors
401 rcc 0.0 8.03  0.0 0.0 -0.31 0.0 2.5
402 rcc 0.0 13.89 0.0 0.0 -0.31 0.0 2.5
403 rcc 0.0 19.75 0.0 0.0 -0.31 0.0 2.5
404 rcc 0.0 25.59 0.0 0.0 -0.31 0.0 2.5
405 rcc 0.0 31.53 0.0 0.0 -0.31 0.0 2.5

c ----------------------------------------------------------------------------
c          MATERIALS
c ----------------------------------------------------------------------------
c Material : MildSteel, mat. ref. no.: 1; rho=0.0852154
m1    6000.     0.00086424
14028.     6.1977e-05
14029.     3.147e-06
14030.     2.0745e-06
25055.     0.00093612
26054.     0.0048717
26056.     0.076475
```

```
26057.     0.0017661
26058.     0.00023504
c Material : Aluminium, mat. ref. no.: 2; rho=0.060261
m2   13027.     0.060261
c Material : Graphite, mat. ref. no.: 3; rho=0.082729
m3    6000.     0.082729
mt3   grph.
c Material : Fuel, mat. ref. no.: 4; rho=0.0597907
m4   13027.     0.058122
92235.     0.001555
92238.     0.00011367
c Material : Aluminium, mat. ref. no.: 5; rho=0.0593267
m5   13027.     0.05908
14028.     7.9083e-05
14029.     4.0156e-06
14030.     2.6471e-06
26054.     9.41e-06
26056.     0.00014772
26057.     3.4114e-06
26058.     4.54e-07
c Material : MildSteel, mat. ref. no.: 6; rho=0.0853705
m6   26054.     0.0048998
26056.     0.076916
26057.     0.0017763
26058.     0.0002364
25055.     0.00063675
6000.     0.00090525
c Material : StainlessSteel, mat. ref. no.: 7; rho=0.0864102
m7    6000.     0.00090525
14028.     0.00078282
14029.     3.975e-05
14030.     2.6203e-05
15031.     4.6177e-05
16032.     2.823e-05
16033.     2.26e-07
16034.     1.2757e-06
16036.     5.9474e-09
24050.     0.00066812
24052.     0.012884
24053.     0.0014609
24054.     0.00036366
```

```
25055.     0.0013625
26054.     0.0033408
26056.     0.052444
26057.     0.0012112
26058.     0.00016118
28058.     0.0064478
28060.     0.0024837
28061.     0.00010796
28062.     0.00034424
28064.     8.7667e-05
42092.     0.00017994
42094.     0.00011216
42095.     0.00019303
42096.     0.00020225
42097.     0.0001158
42098.     0.00029258
42100.     0.00011677
c Material : Concrete, mat. ref. no.: 8; rho=0.0793442
m8    1001.     0.01342
1002.     1.5435e-06
8016.     0.044621
8017.     0.00010869
11023.     0.00094741
13027.     0.0017047
14028.     0.014967
14029.     0.00075999
14030.     0.00050099
19039.     0.00064536
19040.     8.0966e-08
19041.     4.6574e-05
20040.     0.0012402
20042.     8.2772e-06
20043.     1.7271e-06
20044.     2.6687e-05
20046.     5.1173e-08
20048.     2.3923e-06
26054.     1.9965e-05
26056.     0.0003134
26057.     7.2379e-06
26058.     9.6323e-07
c Material : Aluminium
```

```
m101 13027.     0.061308
c Material for RR - Al
m201 13027.10y  1
c -------------------------------------------------------------------------------
c         SOURCE
c -------------------------------------------------------------------------------
sdef erg=d1 vec=0.0 1 0.0 y=d3 z=d4 x=fz=d5
c IAEA STD 2017, A. Carlson et al Nucl.Data Sheets 148(2017)
c 143 Standard n_{th} + U-235 PFNS
c https://www-nds.iaea.org/standards/ref-spectra/PFNS-u235nth.txt
si1 a   0.0000E+00  1.0000E-11  1.5000E-11  2.0000E-11  3.5000E-11
5.0000E-11  7.5000E-11  1.0000E-10  1.5000E-10  2.0000E-10
3.5000E-10  5.0000E-10  7.5000E-10  1.0000E-09  1.5000E-09
2.0000E-09  3.5000E-09  5.0000E-09  7.5000E-09  1.0000E-08
1.5000E-08  2.0000E-08  3.5000E-08  5.0000E-08  7.5000E-08
1.0000E-07  1.5000E-07  2.0000E-07  3.5000E-07  5.0000E-07
7.5000E-07  1.0000E-06  1.5000E-06  2.0000E-06  3.5000E-06
5.0000E-06  7.5000E-06  1.0000E-05  1.5000E-05  2.0000E-05
3.5000E-05  5.0000E-05  7.5000E-05  1.0000E-04  1.5000E-04
2.0000E-04  3.5000E-04  5.0000E-04  7.5000E-04  1.0000E-03
1.5000E-03  2.0000E-03  3.5000E-03  5.0000E-03  7.5000E-03
1.0000E-02  1.3750E-02  1.7500E-02  2.5000E-02  2.6204E-02
2.6828E-02  2.7466E-02  2.8120E-02  2.8789E-02  2.9474E-02
3.0176E-02  3.0894E-02  3.1629E-02  3.2382E-02  3.3152E-02
3.3941E-02  3.4749E-02  3.5576E-02  3.6423E-02  3.7289E-02
3.8177E-02  3.9085E-02  4.0016E-02  4.0968E-02  4.1943E-02
4.2941E-02  4.3963E-02  4.5009E-02  4.6080E-02  4.7177E-02
4.8300E-02  4.9449E-02  5.0626E-02  5.1831E-02  5.3064E-02
5.4327E-02  5.5620E-02  5.6944E-02  5.8299E-02  5.9686E-02
6.1107E-02  6.2561E-02  6.4050E-02  6.5574E-02  6.7135E-02
6.8732E-02  7.0368E-02  7.2043E-02  7.3757E-02  7.5512E-02
7.7310E-02  7.9149E-02  8.1033E-02  8.2961E-02  8.4936E-02
8.6957E-02  8.9027E-02  9.1145E-02  9.3314E-02  9.5535E-02
9.7809E-02  1.0014E-01  1.0252E-01  1.0496E-01  1.0746E-01
1.1001E-01  1.1263E-01  1.1531E-01  1.1806E-01  1.2087E-01
1.2374E-01  1.2669E-01  1.2970E-01  1.3279E-01  1.3595E-01
1.3919E-01  1.4250E-01  1.4589E-01  1.4936E-01  1.5292E-01
1.5655E-01  1.6028E-01  1.6409E-01  1.6800E-01  1.7200E-01
1.7609E-01  1.8028E-01  1.8457E-01  1.8896E-01  1.9346E-01
1.9807E-01  2.0278E-01  2.0761E-01  2.1255E-01  2.1760E-01
2.2278E-01  2.2809E-01  2.3351E-01  2.3907E-01  2.4476E-01
```

2.5059E-01	2.5655E-01	2.6265E-01	2.6891E-01	2.7530E-01
2.8186E-01	2.8856E-01	2.9543E-01	3.0246E-01	3.0966E-01
3.1703E-01	3.2457E-01	3.3230E-01	3.4021E-01	3.4830E-01
3.5659E-01	3.6508E-01	3.7377E-01	3.8266E-01	3.9177E-01
4.0109E-01	4.1064E-01	4.2041E-01	4.3041E-01	4.4066E-01
4.5115E-01	4.6188E-01	4.7287E-01	4.8413E-01	4.9565E-01
5.0745E-01	5.1952E-01	5.3189E-01	5.4454E-01	5.5750E-01
5.7077E-01	5.8435E-01	5.9826E-01	6.1250E-01	6.2707E-01
6.4200E-01	6.5728E-01	6.7292E-01	6.8893E-01	7.0533E-01
7.2211E-01	7.3930E-01	7.5689E-01	7.7490E-01	7.9335E-01
8.1223E-01	8.3156E-01	8.5135E-01	8.7161E-01	8.9235E-01
9.1359E-01	9.3533E-01	9.5759E-01	9.8038E-01	1.0037E+00
1.0276E+00	1.0520E+00	1.0771E+00	1.1027E+00	1.1290E+00
1.1558E+00	1.1833E+00	1.2115E+00	1.2403E+00	1.2698E+00
1.3001E+00	1.3310E+00	1.3627E+00	1.3951E+00	1.4283E+00
1.4623E+00	1.4971E+00	1.5327E+00	1.5692E+00	1.6066E+00
1.6448E+00	1.6839E+00	1.7240E+00	1.7650E+00	1.8070E+00
1.8500E+00	1.8941E+00	1.9391E+00	1.9853E+00	2.0326E+00
2.0809E+00	2.1304E+00	2.1811E+00	2.2330E+00	2.2862E+00
2.3406E+00	2.3963E+00	2.4533E+00	2.5117E+00	2.5715E+00
2.6327E+00	2.6953E+00	2.7595E+00	2.8252E+00	2.8924E+00
2.9612E+00	3.0317E+00	3.1038E+00	3.1777E+00	3.2533E+00
3.3308E+00	3.4100E+00	3.4912E+00	3.5743E+00	3.6593E+00
3.7464E+00	3.8356E+00	3.9269E+00	4.0203E+00	4.1160E+00
4.2139E+00	4.3142E+00	4.4169E+00	4.5220E+00	4.6296E+00
4.7398E+00	4.8526E+00	4.9681E+00	5.0863E+00	5.2074E+00
5.3313E+00	5.4582E+00	5.5881E+00	5.7211E+00	5.8572E+00
5.9966E+00	6.1393E+00	6.2854E+00	6.4350E+00	6.5881E+00
6.7449E+00	6.9055E+00	7.0698E+00	7.2380E+00	7.4103E+00
7.5866E+00	7.7672E+00	7.9520E+00	8.1413E+00	8.3350E+00
8.5334E+00	8.7365E+00	8.9444E+00	9.1572E+00	9.3752E+00
9.5983E+00	9.8267E+00	9.9000E+00	1.0100E+01	1.0300E+01
1.0500E+01	1.0700E+01	1.0900E+01	1.1100E+01	1.1300E+01
1.1500E+01	1.1700E+01	1.1900E+01	1.2100E+01	1.2300E+01
1.2500E+01	1.2700E+01	1.2900E+01	1.3100E+01	1.3200E+01
1.3400E+01	1.3500E+01	1.3700E+01	1.3900E+01	1.4100E+01
1.4200E+01	1.4400E+01	1.4600E+01	1.4950E+01	1.5300E+01
1.5650E+01	1.6000E+01	1.6350E+01	1.6700E+01	1.7050E+01
1.7400E+01	1.7750E+01	1.8100E+01	1.8450E+01	1.8800E+01
1.9150E+01	1.9500E+01	1.9750E+01	2.0000E+01	2.0250E+01
2.0500E+01	2.0750E+01	2.1000E+01	2.1250E+01	2.1500E+01

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2.1750E+01  2.2000E+01  2.2250E+01  2.2500E+01  2.2750E+01
2.3000E+01  2.3250E+01  2.3500E+01  2.3750E+01  2.4000E+01
2.4250E+01  2.4500E+01  2.4750E+01  2.5000E+01  2.5250E+01
2.5500E+01  2.5750E+01  2.6000E+01  2.6250E+01  2.6500E+01
2.6750E+01  2.7000E+01  2.7250E+01  2.7500E+01  2.7750E+01
2.8000E+01  2.8250E+01  2.8500E+01  2.8750E+01  2.9000E+01
2.9250E+01  2.9500E+01  2.9750E+01  3.0000E+01
sp1     0.0000E+00  2.1499E-06  2.6331E-06  3.0405E-06  4.0222E-06
4.8075E-06  5.8880E-06  6.7989E-06  8.3269E-06  9.6151E-06
1.2719E-05  1.5202E-05  1.8619E-05  2.1499E-05  2.6331E-05
3.0405E-05  4.0222E-05  4.8075E-05  5.8880E-05  6.7989E-05
8.3269E-05  9.6151E-05  1.2720E-04  1.5202E-04  1.8619E-04
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3.4463E-01	3.4586E-01	3.4703E-01	3.4813E-01	3.4917E-01
3.5012E-01	3.5101E-01	3.5181E-01	3.5253E-01	3.5317E-01
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3.3231E-01	3.2979E-01	3.2713E-01	3.2433E-01	3.2139E-01
3.1831E-01	3.1508E-01	3.1172E-01	3.0821E-01	3.0457E-01
3.0079E-01	2.9687E-01	2.9281E-01	2.8863E-01	2.8432E-01
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2.5588E-01	2.5075E-01	2.4552E-01	2.4020E-01	2.3480E-01
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1.4208E-01	1.3630E-01	1.3059E-01	1.2493E-01	1.1935E-01
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8.7798E-02	8.2933E-02	7.8199E-02	7.3600E-02	6.9143E-02
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1.8906E-02	1.7065E-02	1.5359E-02	1.3783E-02	1.2332E-02
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4.6642E-05	4.0287E-05	3.4798E-05	2.6933E-05	2.0839E-05
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4.4765E-06	3.4646E-06	2.6809E-06	2.0749E-06	1.6056E-06
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7.4080E-08	6.1687E-08	5.1364E-08	4.2771E-08	3.5614E-08
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3.96499e-20 3.37066e-19 6.43999e-19 5.97235e-19 5.52333e-19 6.06501e-12
2.16188e-11 1.99231e-11 1.86031e-11 1.42243e-08 5.41728e-07 4.82608e-07
4.42484e-07 4.18227e-07 4.34642e-05 5.21665e-05 2.25338e-04 2.87224e-04
8.50129e-04 1.30332e-03 2.11181e-03 3.43792e-03 5.61821e-03 1.16430e-02
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1.99797e-03 1.44126e-03 1.03291e-03 7.73187e-04 5.84797e-04 4.42820e-04
3.43038e-04 2.65853e-04 2.09802e-04 1.62674e-04 1.19929e-04 9.39075e-05
7.84314e-05 6.66049e-05 5.41062e-05 4.57286e-05 3.89881e-05 3.10151e-05
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9.86543e-07 8.00808e-07 7.04148e-07 5.52670e-07 4.79008e-07 3.79424e-07
3.25267e-07 2.71457e-07 2.24891e-07 1.90734e-07 1.62557e-07 1.28654e-07
1.07926e-07 9.06307e-08 7.59531e-08 6.64291e-08
si3 H -0.05 0.15
sp3 D 0 1
si4 a -51.44 -47.63 -40.64 -35.56 -31.75 -19.69 -15.88 -5.29 5.29 15.88
19.69 31.75 35.56 40.64 47.63 51.44
sp4   7.584 7.278 22.16 25.254 40.034 49.608 63.662 68.812 68.812
64.524 50.11 41.86 26.892 24.224 8.946 8.718
c * added by ADVANTG
sb4    6.97987e-05 1.05334e-04 3.56702e-04 8.41244e-04 2.06600e-03 8.90810e-
03
1.49657e-02 3.03418e-02 2.97924e-02 1.49708e-02 4.32663e-03 1.61081e-03
8.91924e-04 3.91739e-04 1.23426e-04 8.15275e-05
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ds5 s 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
si6 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp6   0 0 0 0 0 0 0 0 0 0 0 0 0 2.391 2.525 2.525 2.371 0 0 0 0 0 0 0 0
0 0 0 0 0
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sb6    0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 3.13461e-02 3.70977e-02 3.70021e-02 3.09931e-02 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si7 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp7   0 0 0 0 0 0 0 0 0 0 0 2.496 2.994 2.994 3.15 3.15 2.984 2.984
2.386 0 0 0 0 0 0 0 0 0 0 0
c * added by ADVANTG
sb7    0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 8.88257e-03
9.94343e-03 2.18574e-02 2.65660e-02 2.63963e-02 2.13992e-02 9.49583e-03
8.49915e-03 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si8 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp8   0 0 0 0 0 0 0 0 0 2.685 3.107 3.107 3.685 3.685 3.855 3.855 3.661
3.661 2.979 2.979 2.445 0 0 0 0 0 0 0 0 0
c * added by ADVANTG
sb8    0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 4.16458e-03 4.45353e-03 8.01434e-03
8.51864e-03 2.07880e-02 2.59533e-02 2.61846e-02 2.02245e-02 8.41101e-03
7.63466e-03 4.06736e-03 3.74218e-03 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si9 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
```

```
sp9   0 0 0 0 0 0 0 2.943 3.065 3.065 3.533 3.533 4.177 4.177 4.357
4.357 4.137 4.137 3.395 3.395 2.807 2.807 2.689 0 0 0 0 0 0 0
c * added by ADVANTG
sb9    0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 2.37070e-03 2.47087e-03 3.55656e-03 3.85614e-03 7.28258e-03
7.88342e-03 2.07854e-02 2.71844e-02 2.66334e-02 2.00550e-02 7.72787e-03
6.79182e-03 3.61282e-03 3.31370e-03 2.18256e-03 2.08046e-03 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si10 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp10   0 0 0 0 0 2.877 3.487 3.487 3.637 3.637 4.187 4.187 4.957 4.957
5.149 5.149 4.877 4.877 4.045 4.045 3.381 3.381 3.253 3.253
2.521 0 0 0 0 0
c * added by ADVANTG
sb10   0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 7.58068e-
04
8.21474e-04 1.71358e-03 1.79334e-03 2.74923e-03 2.91059e-03 5.97883e-03
6.54537e-03 2.01876e-02 2.99453e-02 2.95855e-02 1.91316e-02 6.26755e-03
5.68485e-03 2.68087e-03 2.45435e-03 1.59677e-03 1.54213e-03 7.27583e-04
6.39095e-04 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si11 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp11   0 0 0 3.04 3.232 3.232 3.916 3.916 4.086 4.086 4.714 4.714 5.6
5.6 5.802 5.802 5.484 5.484 4.578 4.578 3.864 3.864 3.726 3.726
2.936 2.936 2.75 0 0 0
c * added by ADVANTG
sb11   0.00000e+00 0.00000e+00 0.00000e+00 4.29082e-04 4.32715e-04 7.07406e-
04
7.95794e-04 1.61103e-03 1.69287e-03 2.61672e-03 2.91778e-03 5.97645e-03
6.50968e-03 1.93912e-02 3.03044e-02 2.93746e-02 1.94334e-02 6.20761e-03
5.71663e-03 2.65618e-03 2.41607e-03 1.61096e-03 1.51400e-03 7.34233e-04
6.49049e-04 3.98141e-04 3.83828e-04 0.00000e+00 0.00000e+00 0.00000e+00
si12 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp12   0 2.823 3.229 3.229 3.421 3.421 4.147 4.147 4.331 4.331 5.007
```

```
5.007 5.975 5.975 6.183 6.183 5.835 5.835 4.893 4.893 4.153
4.153 4.015 4.015 3.199 3.199 3.007 3.007 2.495 0
c * added by ADVANTG
sb12   0.00000e+00 2.02446e-04 2.20243e-04 3.72534e-04 3.70077e-04 6.10445e-
04
6.99731e-04 1.53430e-03 1.52600e-03 2.42917e-03 2.69763e-03 5.68409e-03
6.11274e-03 1.91718e-02 3.05423e-02 3.10833e-02 1.93183e-02 5.66694e-03
5.27569e-03 2.44712e-03 2.27978e-03 1.42032e-03 1.40427e-03 6.05367e-04
5.64403e-04 3.37401e-04 3.19580e-04 1.94757e-04 1.73774e-04 0.00000e+00
si13 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp13   0 2.926 3.338 3.338 3.516 3.516 4.27 4.27 4.458 4.458 5.172
5.172 6.196 6.196 6.412 6.412 6.042 6.042 5.084 5.084 4.336
4.336 4.204 4.204 3.38 3.38 3.194 3.194 2.67 0
c * added by ADVANTG
sb13   0.00000e+00 1.12126e-04 1.20549e-04 2.09436e-04 2.15064e-04 3.86203e-
04
4.34884e-04 1.06840e-03 1.09089e-03 1.78638e-03 1.97705e-03 4.63300e-03
5.10037e-03 1.92721e-02 3.44113e-02 3.27288e-02 1.79152e-02 4.79846e-03
4.29640e-03 1.83959e-03 1.70778e-03 9.86140e-04 9.86939e-04 4.01027e-04
3.46298e-04 1.95507e-04 1.90489e-04 1.10557e-04 9.65784e-05 0.00000e+00
si14 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp14   0 2.843 3.237 3.237 3.407 3.407 4.131 4.131 4.315 4.315 5.005
5.005 6.005 6.005 6.215 6.215 5.853 5.853 4.921 4.921 4.197
4.197 4.069 4.069 3.277 3.277 3.099 3.099 2.601 0
c * added by ADVANTG
sb14   0.00000e+00 2.04582e-04 2.17539e-04 3.60582e-04 3.67105e-04 6.19891e-
04
6.83301e-04 1.50593e-03 1.52396e-03 2.41361e-03 2.63809e-03 5.66135e-03
6.05570e-03 2.02538e-02 3.10031e-02 3.04373e-02 1.88340e-02 5.68531e-03
5.20092e-03 2.44361e-03 2.30566e-03 1.44873e-03 1.43398e-03 6.36945e-04
5.68848e-04 3.39479e-04 3.30695e-04 2.04023e-04 1.83983e-04 0.00000e+00
si15 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
```

```
sp15   0 0 0 3.066 3.234 3.234 3.916 3.916 4.09 4.09 4.734 4.734 5.67
5.67 5.87 5.87 5.528 5.528 4.632 4.632 3.932 3.932 3.814 3.814
3.048 3.048 2.892 0 0 0
c * added by ADVANTG
sb15   0.00000e+00 0.00000e+00 0.00000e+00 4.14157e-04 4.49399e-04 6.86324e-
04
8.03235e-04 1.57168e-03 1.73275e-03 2.60360e-03 2.94240e-03 5.83516e-03
6.28678e-03 2.09661e-02 3.07414e-02 2.91704e-02 1.84333e-02 6.14810e-03
5.51159e-03 2.65333e-03 2.47575e-03 1.56118e-03 1.52587e-03 7.09904e-04
6.40321e-04 4.00666e-04 3.94810e-04 0.00000e+00 0.00000e+00 0.00000e+00
si16 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp16   0 0 0 0 0 2.942 3.556 3.556 3.714 3.714 4.284 4.284 5.108 5.108
5.286 5.286 4.974 4.974 4.136 4.136 3.478 3.478 3.366 3.366
2.652 0 0 0 0 0
c * added by ADVANTG
sb16   0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 1.02032e-
03
1.12142e-03 2.14148e-03 2.21836e-03 3.29112e-03 3.62233e-03 6.90514e-03
7.46673e-03 2.06749e-02 2.77478e-02 2.69418e-02 1.98501e-02 7.02426e-03
6.41219e-03 3.25870e-03 3.03847e-03 2.03247e-03 1.98650e-03 1.01126e-03
8.87188e-04 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si17 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp17   0 0 0 0 0 0 0 3.115 3.257 3.257 3.743 3.743 4.441 4.441 4.587
4.587 4.305 4.305 3.545 3.545 2.935 2.935 2.837 0 0 0 0 0 0 0
c * added by ADVANTG
sb17   0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 2.39481e-03 2.47584e-03 3.66645e-03 3.82492e-03 7.38734e-03
7.93733e-03 2.03563e-02 2.75693e-02 2.65352e-02 2.00493e-02 7.42430e-03
6.84741e-03 3.63284e-03 3.23116e-03 2.09693e-03 2.13830e-03 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si18 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp18   0 0 0 0 0 0 0 0 0 2.957 3.395 3.395 4.027 4.027 4.149 4.149
```

```
3.881 3.881 3.177 3.177 2.603 0 0 0 0 0 0 0 0 0
c * added by ADVANTG
sb18   0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 4.19223e-03 4.49038e-03 7.93155e-03
8.79667e-03 2.13269e-02 2.64594e-02 2.57388e-02 1.99326e-02 8.14892e-03
7.47157e-03 4.06976e-03 3.69825e-03 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si19 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp19   0 0 0 0 0 0 0 0 0 0 0 0 2.891 3.455 3.455 3.537 3.537 3.271 3.271
2.679 0 0 0 0 0 0 0 0 0 0 0
c * added by ADVANTG
sb19   0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 9.31114e-03
9.96251e-03 2.21271e-02 2.69738e-02 2.60838e-02 2.07962e-02 9.24293e-03
8.39024e-03 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
si20 a -52.26 -52.24 -49.09 -49.07 -45.93 -45.91 -39.59 -39.57 -36.43
-36.41 -30.09 -30.07 -14.26 -14.24 -4.75 4.75 14.24 14.26 30.07
30.09 36.41 36.43 39.57 39.59 45.91 45.93 49.07 49.09 52.24
52.26
sp20   0 0 0 0 0 0 0 0 0 0 0 0 0 0 2.952 2.994 2.994 2.736 0 0 0 0 0 0 0
0 0 0 0 0 0
c * added by ADVANTG
sb20   0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 3.26349e-02 3.75481e-02 3.62787e-02 3.02492e-02 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00 0.00000e+00
c ------------------------------------------------------------------------------
c          TALLIES
c ------------------------------------------------------------------------------
f4:n     101 103 104 105
f114:n   101 103 104 105
fm114:n  1 201 107
c --------------- PHYSICS CARDS --------------------------
mode n
cut:n  j 3
NPS 1e8
```

```
rand gen=2 seed=501932527452171 stride=152917 hist=1
c * added by ADVANTG
wwp:n 5.0 j 100 j -1 0 1.018748353e+00
nonu
```

C List of all appended MCNP input files and WW files

The list includes separate MCNP input files (*.i) for each of the detectors (s - Sulphur, in - Indium, rh - Rhodium, au - Gold, al - Aluminium) and their corresponding weight-window files (*.wwinp). The input for the gold activation foil does not include variance reduction parameters and an additional WW file at this point.

```
aspis-fe88_in.i
aspis-fe88_rh.i
aspis-fe88_s.i
aspis-fe88_al.i
aspis-fe88_au.i
aspis-fe88_rh.wwinp
aspis-fe88_in.wwinp
aspis-fe88_al.wwinp
aspis-fe88_s.wwinp
```

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