ISSN 1977-5296

ESARDA

European Safeguards Research and Development Association

Bulletin

Nº 42

Non-Destructive Analysis
Special Issue

November 2009

ISSN 1977-5296

Number 42
November 2009

ESARDA is an association formed to advance and harmonize research and development for safeguards. The Parties to the association are:
Areva, France
ATI, Austria
BNFL, United Kingdom
CEA, France
CNCAN, Romania
EDF, France
ENEA, Italy
European Commission
FZJ, Germany
HAEA, Hungary
IKI, Hungary
IRSN, France
MITyC, Spain
NRPA, Norway
SCK/CEN, Belgium
Sellafield Ltd, United Kingdom
SFOE, Switzerland
Springfields Fuels Limited, United Kingdom
SSM, Sweden
STUK, Finland
UKAEA, United Kingdom
VATESI, Lithuania
WKK, Germany

Editor
C. Versino on behalf of ESARDA
EC, Joint Research Centre
T.P. 210
I-21020 Ispra (VA), Italy
Tel. +39 0332-789603, Fax. +39 0332-789185
esarda-bulletin@jrc.it

Scientific and technical papers submitted for publication are reviewed by the Editorial Committee.

Manuscripts are to be sent to the Editor following the 'instructions for authors' available on the 'Bulletin' page of the ESARDA website. Photos or diagrams should be of high quality.

Accepted manuscripts are published free of charge.

N.B. Articles and other material in ESARDA. Bulletin do not necessarily present the views or policies of ESARDA nor of the European Commission.

ESARDA Bulletin is published jointly by ESARDA and the Joint Research Centre of the European Commission.
It is distributed free of charge.

The publication is authorized by ESARDA.

Cover designed by
N. Bähr
EC, JRC, Ispra, Italy

Printed by
IMPRIMERIE CENTRALE – Luxembourg

ESARDA
European Safeguards Research and Development Association

Bulletin

Table of Content issue n° 42

Editorial

Special Issue on Non Destructive Analysis

P. Peerani
European Commission, Joint Research Centre

In June 2006, the ESARDA Bulletin published as Issue number 34 the first of the Bulletin's Special Issues. Special Issues are published occasionally, in addition to the two regular Bulletins published per year, and have a monographic character, being the entire number dedicated to a specific and single topic.

The first Special Issue was dedicated to NDA and contained the final report of the ESARDA Multiplicity Benchmark (at that time dealing with phases I and II). After three years we are back with a Special Issue entirely dedicated to two products of the ESARDA NDA Working Group:

- the report of the III and IV phases of the ESARDA Multiplicity benchmark;
- the Good Practice Guide for the use of Modelling Codes in Non Destructive Assay of Nuclear Materials.

The first paper describes the continuation of the project that made the subject of the previous Special Issue. Benchmarking is a common procedure in applied science in order to assess and validate methodologies, techniques or components (either instruments or software). The ESARDA Multiplicity Benchmark had a two-fold goal:

- test and validate Monte Carlo codes in the simulation of neutron multiplicity counters;
- test and validate LIST-mode data acquisition software for the processing of time-stamped pulse trains.

For this reason, already at the initial step the benchmark had been split in two phases: one aiming to compare full Monte Carlo modelling of a neutron multiplicity system, the second aiming to compare data processing codes for the analysis of acquired LIST-mode data. At the time of the first exercise launched in 2003, LIST-mode acquisition system were still under development, so the first exercise was focussed to a series of theoretical cases: so the Monte Carlo simulations were benchmarked against theoretical point-model mathematical solutions and the processing codes were applied to synthetic pulse trains produced by Monte Carlo simulations.

When the first hardware developments were completed at some research laboratories, the first neutron counting systems with LIST-mode data acquisition become available and the NDA working group sponsored a series of experimental campaigns performed during 2006 and 2007 at the PERLA laboratory of JRC to compare some systems. These campaigns made available a set of experimental data that were used as a basis for the continuation of the exercise. The III and IV phases of the multiplicity benchmark consist respectively in the comparison of full Monte Carlo simulations and LIST-mode pulse train analysis with experimental data. The results of this exercise make the subject of the report in this Bulletin.

The second paper focuses on a subject partly in common with the previous one, Monte Carlo simulation. This technique has become more and more frequently used as a complementary tool in NDA measurements, in particular replacing experimental calibration when suitable reference material are not available. The introduction of numerical calibration in safeguards procedures had initially to win the reluctance of many sceptics, but an extensive effort of validation (also through several benchmarks organised by the ESARDA NDA working group) and the success of the first trial cases allowed finally to have this technique accepted by IAEA and Euratom.

Once Monte Carlo became a standard technique, the nuclear safeguards community realised the need to establish common and clear rules on the application of Monte Carlo modelling. In particular the IAEA stimulated the NDA working group to develop a good practice guide (GPG) in numerical simulation on a similar basis of GPG's used in the other (experimental) measurement techniques. The document presented in this Bulletin results from the contributions of several Monte Carlo experts of the NDA working group and provides a set of recommendations of best practices in the application of numerical simulation and modelling of NDA techniques.

Scientific articles

ESARDA Multiplicity Benchmark Exercise – Phases III and IV

P. Peerani[1], M. Swinhoe[2], A-L. Weber[3], L. G. Evans[4]
1. European Commission, Joint Research Centre, IPSC – Ispra (VA), Italy
2. Institut de Radioprotection et Surete Nucleaire, Fontenay-aux-Roses, France
3. N-1, Safeguards Science and Technology Group, LANL – Los Alamos (NM), USA
4. University of Birmingham, Canberra – Meriden (CT), USA
E-mail: paolo.peerani@jrc.it

Abstract

In 2003 the ESARDA NDA working group launched a benchmark exercise in order to compare the different algorithms and codes used in the simulation of neutron multiplicity counters. The results of the 1st and 2nd phase of the ESARDA Multiplicity Benchmark, based on synthetic cases, have been published in the ESARDA Bulletin number 34. Notwithstanding the satisfactory conclusion that all the algorithms developed by the different participants in the first two phases and used to analyse the pulse trains have proven to be satisfactory, the working group felt that an extension to real experimental cases would have added a supplementary value to the exercise that brought to the organisation of phases III and IV. This paper summarises the outcomes of the benchmark, whose full report will soon be made available on the ESARDA Bulletin.

Keywords: NDA, neutron counting, neutron multiplicity, Monte Carlo.

1. Rationale

In 2003 the ESARDA NDA working group launched a benchmark exercise in order to compare the different algorithms and codes used in the simulation of neutron multiplicity counters. In order to derive the maximum amount of information and at the same time to allow a large participation, the working group decided to split the exercise into two parts with two participation levels: a full simulation exercise where participants were asked to compute the count rates starting from the basic technical specifications and/or a partial exercise involving the processing of the pulse trains produced by a single laboratory. The results of participants performing the entire exercise enabled a comparison among the different Monte Carlo codes for the simulation of neutron multiplicity counters. The results of the partial exercise help to test the available algorithms for pulse train analysis and to derive some important information about the models applied for dead-time correction. The results of the 1st and 2nd phase of the ESARDA Multiplicity Benchmark have been published elsewhere [1, 2].

All the cases run in the first two phases of the benchmark were theoretical. So the conclusions derived had to be considered as a relative behaviour of the different models, techniques and codes. Notwithstanding the satisfactory conclusion that all the algorithms developed by the different participants in the first two phases and used to analyse the pulse trains have proven to be satisfactory, the working group felt that an extension to real experimental cases would add value to the exercise.

First of all it would provide a further validation to the Monte Carlo codes such as MCNPX, MCNP-PTA or MCNP-Polimi in the specific field of neutron correlations. In fact to our knowledge, there has been no other case of a benchmark comparing Monte Carlo to experiments on neutron correlations, except the previous ESARDA exercise and even in that case the comparison was limited to Reals (or Doubles) counting [3]. A complete assessment with comparison of calculated and measured Singles, Doubles and Triples would be accomplished through the 3rd phase of the ESARDA Multiplicity Benchmark.

A more practical consideration brings us to the justification of the 4th phase. Nowadays most of the neutron counting systems is based on feeding a train of TTL logic pulses into a neutron analyser performing the time correlation analysis. In future these systems could be replaced by the introduction of time-stamped data acquisition cards that replace the logical pulse by a digital time stamp (LIST mode acquisition). These digital pulse trains could be directly fed to an acquisition computer and processed by software, without further need for an additional hardware component, such as an (ordinary or Mul-

tiplicity) Shift Register Analyser. This could be the future major development in practical neutron correlation analysis, given data transfer rates, storage and analysis criteria can be met. There are potential secondary benefits: e.g. more robust monitoring of the state of the health of the equipment; the potential for continued operation with revised calibration parameters given failure of a sub-set of detectors; access to alternative analysis methods; a complete record of the data; refined fault finding capability etc. The programs developed by the participants to the 2nd phase of the ESARDA Multiplicity Benchmark can be used directly and without any modification to process the digital pulse trains produced by experimental measurements performed in LIST mode. The main aim of this exercise is to test and validate the LIST mode operation of neutron multiplicity counters against the established practice.

2. Description of the exercise

The measurements have been performed in the PERLA laboratory at the JRC site of Ispra (Italy) using an Active Well Coincidence Counter (AWCC), see Figure 1. All the acquisitions were repeated using:

- a conventional multiplicity shift register analyser (CANBERRA 2150)
- a Multi-Event Datation System card (MEDAS from Cesigma)

The count rates acquired with the 2150 and analysed with the INCC software will be considered the reference to which the results will be compared.

The following item measurements have been used in the exercise:

1. Californium source of low intensity
2. Californium source of high intensity
3. Small Pu metal sample
4. Pu oxide sample of small mass
5. Pu oxide sample of large mass
6. MOX sample

The experimental pulse trains were generated by a MEDAS card provided by IRSN [4]. The MEDAS card produces a binary file listing the time intervals between two successive detection events. This file was converted in order to produce a LIST mode pulse train with absolute time sequence. At the same time the format was converted to ASCII. The files that were distributed for the 4th phase were then text files with sequence of detection times. Being an experimental acquisition, the time sequence will be correctly always increasing, avoiding the problem occurred with the simulated file and not requiring the rearrangement of values needed in the previous exercise. Moreover the dead-time effect from the resolving time of the charge amplifier/dis-

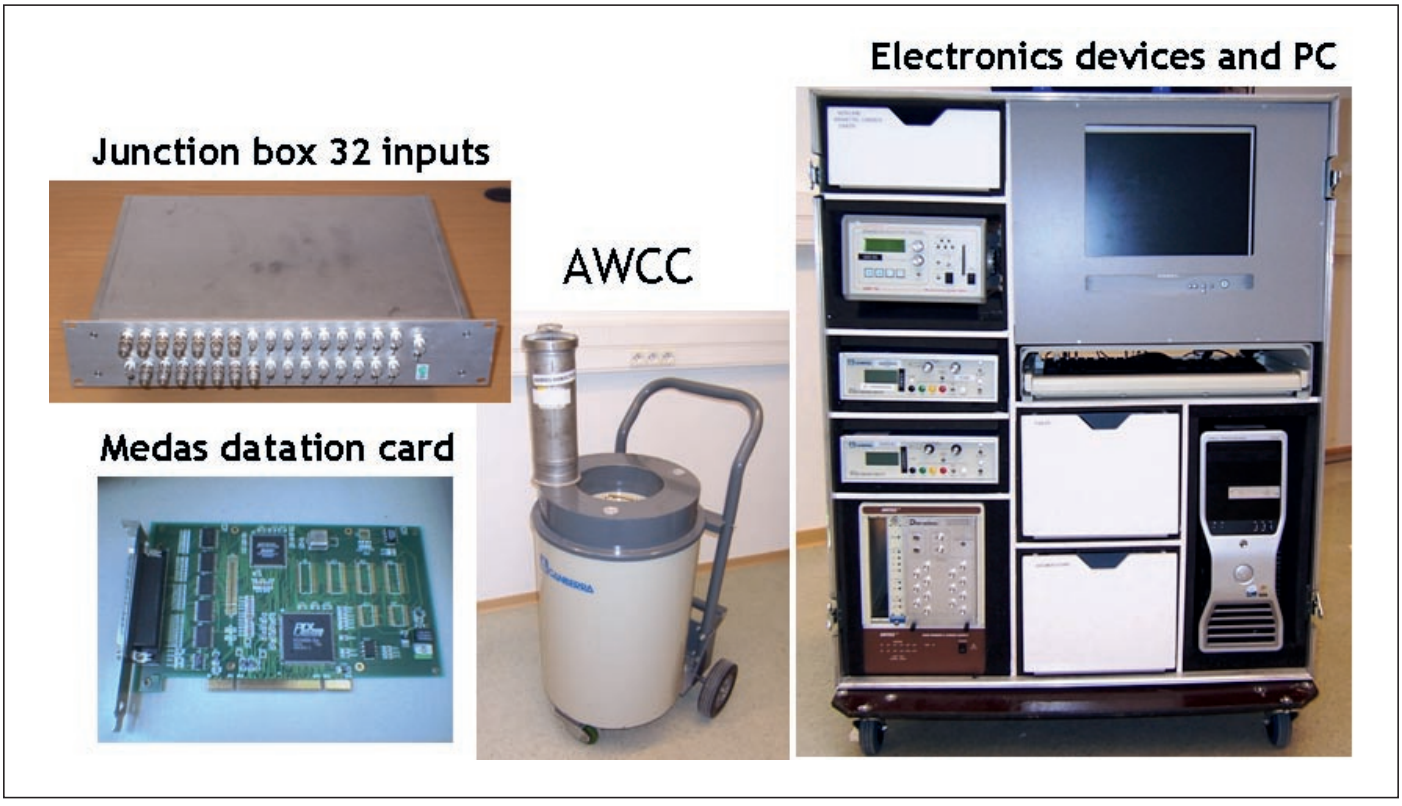


Figure 1: Experimental setup.

criminator boards and subsequent stages of electronic processing is embedded in the measurement chain, so the participants were not asked to remove counts in order to simulate dead-time effects.

3. Specifications for the pulse train generation

The detector used was an Active Well Coincidence Counter (AWCC) in fast configuration (Cd liner inside the cavity) with both disks removed (cavity height 35 cm) [5]. This corresponds to the specification of the one used in the 1st phase avoiding the participants the effort to develop a new detector model. Only the samples had to be modelled according to the detailed description provided below.

3.1. Case 1 – Cf source of low intensity

This case refers to the measurement of a Cf-252 source placed at the centre of the AWCC cavity. Geometrically the source is a very small piece of metal wire and to all effects can be considered point-like. It is contained in a cylindrical stainless steel capsule with an external radius of 0.4 cm, height of 1 cm and wall thickness of 0.13 cm. The intensity of the source (6005-NC) was certified by NPL and after decay correction it results to be 3781 n/s at the measurement date (with a 1-sigma uncertainty of about 1%).

3.2. Case 2 – Cf source of high intensity

The case refers to a geometrical configuration identical to case 1. The only difference is the intensity of the source (6001-NC) that was 497200 n/s at the measurement date (with a 1-sigma uncertainty of about 1%).

3.3. Case 3 – Pu metal sample

The case refers to the measurement of a plutonium metal sample (PERLA-211), indeed a PuGa alloy with 1.5% Ga. The geometry is a thin (0.6 mm) metal disk and an approximate diameter of 3.3 cm. It was placed horizontally at the cavity mid-plane (17.5 cm from the bottom). The plutonium certified mass was 9.455 g, the isotopic composition was 0.13% Pu-238, 75.66% Pu-239, 21.49% Pu-240, 1.95% Pu-241 and 0.77% Pu-242, the Am/Pu ratio was 0.0186, all data referred to July 1996.

3.4. Case 4 – Pu oxide sample of small mass

The sample was the PERLA sample 102, being a PuO_2 powder with an estimated density of 2.6 g/cm^3 contained in a model-200 container. The plutonium certified mass was 51.455 g (59.13 g of powder), the isotopic composition was 0.199% Pu-238, 70.955% Pu-239, 24.583% Pu-240, 3.288% Pu-241 and 0.975% Pu-242, the Am/Pu ratio was 0.0102, all data referred to November 1987. The container is constituted by two shells: an inner cylinder in AISI-304 stainless steel wrapped in a polyurethane bag (this latter can be neglected in the model), all inserted in an outer cylindrical box also in AISI-304 stainless steel, sealed with steel bolts. A 10-cm high aluminium spacer was used to place the sample at the centre of the measurement cavity.

3.5. Case 5 – Pu oxide sample of large mass

The sample was the PERLA sample 111, also a PuO_2 powder, having the same density and isotopic composition of sample 102, only the total mass and container type change. The plutonium certified mass was 999.825 g (1148.96 g of powder), always referred to November 1987. The container was a model-1000, similar in shape and composition to the previous one, only having larger dimensions. It was placed at the bottom of the AWCC cavity.

3.6. Case 6 – MOX sample

The sample was the PERLA sample ENEA01. This is a MOX powder contained in a model-2500 container placed at the bottom of the AWCC cavity. The net MOX powder mass is 1011.13 g, of which 675.4 g is uranium and 168.151 g is plutonium. The density is significantly lower than the PuO2 powder and was estimated to be 0.7÷0.9 g/cm3. Uranium enrichment is natural, whereas the plutonium isotopic composition was 0.17% Pu-238, 66.54% Pu-239, 28.02% Pu-240, 3.26% Pu-241 and 2.01% Pu-242, the Am/Pu ratio was 0.0081, data referred to December 1988.

4. Results from full simulations

The scope of this part of the exercise is to have a comparison of the different codes available for the complete simulation of a neutron multiplicity counter. Six laboratories provided results for the full exercise.

The laboratories are more or less the same who participated to the phase 1 and they used the same codes: MCNPX by LANL and IRSN, MCNP-PTA by JRC, MCNP-PoliMi by Chalmers and Univ. Michigan and MCNP+AM technique by IPPE. A new participant, IRSN, provided two sets of results: one with MCNPX with direct calculation of moments, the second by generating pulse trains with MCNPX and then processing the files with the post-proces-

sor TRIDEN, used also for phase 4. Methodological details have been already described in [1] and will not be repeated here.

a) Zero dead-time

Table 1 shows the comparison of the simulation results in an ideal case of zero dead-time. The quoted uncertainties are purely statistical at 1-sigma level. In this case the calculated values can be compared with the theoretical value computed using the point model [6]. The results are also reported in graphical form on plots shown in Figures 2a to 2f; for practical reasons in these plots the point model value was set as reference to 1 even though there is no evidence that this can be assumed as a "true value". In the axis the participants are labelled from 1 to 6 according to the same order of Table 1.

It is worthwhile to note that comparison to the point model is not trivial, because it requires the knowledge of parameters like the efficiency, the leakage multiplication and the gate utilisation factors. The Pu sources are confounded by (alpha,n) neutrons with a different energy distribution and a finite extent which may violate the strict assumptions of the point model, but more importantly the items were not all measured in the same position so there will be a shift in efficiency from the centre to the floor. Some variants of the point model may imply a simple exponential die-away and the AWCC is not truly ideal in that sense. The "reference" values reported in Table 1 have been computed applying the point model equations with some simplifications and approximations. The values for efficiency and multiplication were derived from the Monte Carlo calculations; this automatically accounts for variation of efficiency within the cavity, size and shape of the sample, different energy of neutrons from (alpha,n) and spontaneous fission. The doubles gate fraction was computed assuming a single exponential with an approximate die-away time of 50 μs and the triples gate fraction was assumed to be the square of the doubles gate fraction. The moments of the induced fission multiplicity distributions were taken from fast (1 MeV) neutron fission, not from thermal fission as often used.

The results of the simulations at zero dead-time show an excellent agreement among the different participants, with standard deviations within a few percent in most of the cases. It is true that all the methods have a common model for the simulation of neutron transport based on MCNP, but the methods differ on the treatment of time correlations and in any case we always expect some effects linked to the human factor (the way in which the user models the system). Taking all this into account the agreement among the results is satisfying.

Even though there is no clear evidence of strong systematic errors, some clear trends are visible. For instance all the results based on MCNPX tend to be consistently lower than those based on MCNP-Polimi; MCNP-PTA tends to overestimate Triples, whereas IPPE method tends to underestimate them.

Moreover the agreement between simulations, theoretical expectations and measurements are also good. This confirms the applicability of the point model in the cases represented in this exercise.

b) Dead-time effects

The previous data cannot be directly compared with measurements, since measured data are affected by dead-time effects. So we have two possibilities, either we correct the measured data in order to derive zero dead-time values or the dead-time effects should be included in the simulation. Dead-time corrected experimental values have been also included in Table 1 and can be compared with the zero dead-time simulations there. In this section we have considered the second option.

MCNP-PTA allows direct modelling of dead-time for each component of the electronic chain (amplifiers and OR-chain or mixer), MCNPX can produce a pulse train file that can be post-processed by a simulation program that includes dead-time effects (in case of IRSN the TRIDEN software uses a global system dead-time). Both codes apply a paralysable dead-time model. JRC used a dead-time component of 1 μs per each of the 6 amplifiers and 20 ns for the OR-chain; this corresponds to a system dead-time of 1000/6+20 = 187 ns, consistent with the one used by IRSN (170 ns). Therefore IRSN and JRC provided as well a set of results that can be directly compared with measured values. This is reported in Table 2.

When comparing simulations with measurements, we notice a less close agreement. This can only be marginally attributed to the uncertainty introduced by dead-time effects, or the way how the dead-time is modelled. There is certainly some unresolved inconsistency between the model and the reality. This is espe-

cially true for the low count rate cases where the dead-time correction is negligible. This is confirmed by the comparison of the dead-time corrections (obtained by dividing the results of Table 1 by those of Table 2) shown in Table 3.

By consequence we have to attribute the origin of the discrepancies to modelling and, to a less extent, to the nuclear data used by the two codes. Indeed we have to keep in mind that the PERLA standards are certified with a very high precision in terms of mass and isotopic composition, but much less in terms of their geometrical properties. Container size is of course known, but there is a large uncertainty on the powder density of cases 4, 5 and 6 that is reflected on an uncertainty of the filling height and therefore on the actual sample dimensions. This affects quite strongly the multiplication and therefore introduces a systematic error that increases with the order of the moments. Especially in case 6 the density of MOX powder is not known at all (explaining the strong discrepancies in this case), whereas the density of PuO2 (assumed to be 2.6 g/cm3) has been obtained using some gamma scanning of the containers that allowed us to derive the powder filling height with reasonable accuracy. A similar consideration applies to case 3 where the sample thickness is not certified.

5. Results from pulse train analysis

The LIST mode files processed from the MEDAS card acquisitions have been distributed to the participants, who were requested to compute the Singles, Doubles and Triples counting rates for all the pulse trains. For each case 1000-second acquisitions were performed, more precisely ten independent acquisitions of 100 seconds. The participants produced the S, D and T count rates (average on the ten short acquisitions) together with their absolute uncertainties. Additionally they were requested to provide indicative processing times of the pulse trains together with the PC characteristics.

The same consideration about the methodology applies to phase 4, where the participants used the same tools as in phase 2 and therefore they are fully described in the final report of the first two phases [1].

All the results are reported in tabular form in Table 4 and graphically in Figures 3a to 3f. Generally the agreement among the different processing codes is extremely good: negligible deviations in Singles (less than 0.1%), agreement within 0.1%-0.4% in Doubles. Nevertheless dispersion up to 4% in Triples is visible, indicating that the way to compute them is not totally homogeneous.

The values can also be compared to the measured S, D, T with a multiplicity shift register. Indeed it is one of the scopes of the exercise to assess the capability of LIST mode acquisition to correctly collect the measured data in view of a possible alternate technology in time-stamped data acquisition for neutron counting applications. Indeed the results show that data acquired with the data acquisition card and processed with all the tested codes agree with the multiplicity shift register data within the statistical uncertainties. We should bear in mind that the shift register measurements and the LIST mode measurements were done with the same experimental setup, but sequentially in time. This means that they do not refer exactly to the very same pulse train, but to two sequential pulse trains acquired in identical conditions. Also it is possible that the shift register and List Mode units introduce slightly different dead-times. So we can only conclude that they coincide within the statistical uncertainty and no systematic deviations have been revealed. We remind that the “measured” data reported in Table 4 refer to the raw values provided by multiplicity shift register without any correction (neither dead-time nor background).

Observation of the data in Table 4 reveals that the assessment of uncertainties in the mean count rates varies between participants. As reported above, the relative standard deviations in the mean count rates vary up to a maximum of 4% for Triples, however the deviations in the uncertainty estimates themselves are significantly greater. A deviation of up to 460% has been observed in the calculated uncertainties, relative to the measured uncertainties. The greatest dispersion in uncertainty estimates between participants was for the uncertainties in the mean Triples rates for case 2 with the highest source intensity.

Three summary plots are given in Figure 4 to show the measured Singles, Doubles and Triples count rates, in ascending order of count rate, for each of the six source cases. It is then of interest to plot the Singles, Doubles and Triples rates for each of the cases individually to illustrate trends in the data and the magnitude of differences in the uncertainty estimates between participants. The measured and calculated Singles, Doubles and Triples rates have been plotted for each of the six source cases in Figures 5a, 5b and 5c, respectively. Clear trending in the distribution of uncertainties can be observed in these three figures. Participant laboratory CEA-DAM had consistently higher uncertainty estimates than other participants. This can be explained by

the fact that reported uncertainties for CEA-DAM were quoted as two standard deviations of the mean count rates. It has therefore been deemed necessary to document how uncertainties were calculated. All participants were asked to provide a detailed method of how they calculated the uncertainties on the Singles, Doubles and Triples rates. Calculation methods from individual participant groups have been reported in Appendix.

The S, D and T rates from each group have been plotted in ascending order (from lowest to highest) on 3 curves, along with the reported uncertainty values to see if any further trending in the data can be observed. This also provides a visual check as to whether one participant is consistently low or high in reporting uncertainties – see Figure 4.

A further point of interest is the processing time required which varies by more than an order of magnitude. This will be partly due to the computer processing power available but there may also be tips and tricks that could benefit the safeguards community, if, as we expect, there is widespread future use of list mode data. For instance IKI processing code is systematically the fastest; this could be due to the use of integer mathematics, which is much faster than using floating point numbers. JRC post-processing code had an evolution during the exercise that reduced his running time of more of an order of magnitude, just by optimising the programming (compare results JRC and JRC-2 in Table 4).

6. Conclusions

The results presented here lead to a number of interesting and important conclusions. There are two separate topics. The first is the simulation of measurements using Monte Carlo. In this area the results of the different participants are very similar. However differences do remain. This is in spite of the fact that the basic geometric model was the same in all cases. A close comparison of the input/output files used by the participants will reveal the sources of these differences. The effect of input parameters such as fill height or nuclear data is available in these results and could lead to useful information on the accuracy of simulations for Monte Carlo users.

The second part of the work involved the analysis of pulse trains. In this area also the results from the different participants are very similar. The difference between the results is small for most practical purposes. However when one considers that each team was starting from identical pulse trains it seems that further detailed comparison of the algorithms used would be warranted. One free parameter in the analysis is the length of the long delay and another difference is how the physical end of the data is treated. Otherwise the results would be expected to be truly identical. A study of the different data treatment algorithms could be used to establish a reference standard for the data analysis.

One outstanding feature of these results is the quoted absolute error. The values appear to vary by an order of magnitude from group to group. This is an important issue that again should be studied by a more detailed comparison of the calculation methods and even definitions of uncertainty used by the different groups. The results could be compared to the values from the shift register electronics and theoretical values. We just underline that from a theoretical point of view the statistical uncertainty of a measurement should not depend on the fact that the acquisition is done using a shift register or LIST mode.

Overall, the results of this exercise show that all participants are capable of good performance for practical purposes. However, comparison of the methods used by the different groups should allow the establishment of more robust analysis techniques with more reliable error estimates.

Appendix – calculation of uncertainties

Here we will report the methods used by some of the participants to estimate the uncertainties based on information provided by the authors:

JRC:

The quoted uncertainty is the sample standard deviations for counting rates computed using the 10 results of the individual runs.

Birmingham/ Canberra Method (L. Evans):

In each of the 6 cases, the MSR analysis was completed for each of the 10 pulse trains. Each of the 10 pulse trains (approximately 100 seconds in length) were further divided into 10 segments of approximately 10 seconds in duration, then 20 cycles of approximately 5 seconds in duration. The purpose of this segmented pulse train analysis was to enable the estimation of the dispersion in the mean rates, based on replicate counting of an assay item.

The mean S, D and T rates quoted in the spreadsheet were calculated by the following method:

- S, D & T rates were calculated for each cycle
- Average S, D & T rates were calculated for each pulse train by summing rates from each of the cycles and dividing by the number of cycles.

- The final mean rates quoted for each source are the average of the S, D & T rates from each of the 10 pulse trains.

The uncertainty in each of the mean rates is expressed as the standard error, representing the spread in the mean rates over the 10 (or 20 segments as appropriate). Again, the standard error quoted in the final results is an average uncertainty over each of the 10 pulse trains.

CEA-DAM (R. Oddou):

The calculated uncertainties is equal the twice standard deviation of the 10 values

S = mean(Si) (i = 1 to 10)
S abs unc = 2 * standard deviation (Si) (i = 1 to 10)
The same was done for D and T.

Note: in order to make the results consistent with the other participants, the CEA-DAM results reported in Table 4 and in Figures 3 are those provided by the author divided by two.

Chalmers (B. Dahl):

The uncertainty given was calculated as the standard deviation according to the formula

$$\sqrt{\frac{1}{9}\sum_{i=1}^{10}(x_i - \bar{x})^2}$$

where $\bar{x}$ is the mean value and x_i are the values from the 10 different sets.

IPPE (V. Nizhnik):

Two methods were used: the first estimates counting rate random errors based on sample standard deviation upon 10 cycles (pulse-trains). The second one is based on theoretical standard deviation estimation derived from summarized SR multiplicity distribution. For these calculations we used procedures described in [B. Harker, M. Krick: “INCC Software Users Manual”, LA-UR-99-1291 (July1998)].

Both methods showed good agreement for Singles and Doubles counting rates, but at the same time, big discrepancy was observed between these two methods for Triples.

References

[1] P. Peerani: “ESARDA Multiplicity Benchmark Exercise – Final report”, ESARDA Bulletin, Nr. 34, June 2006, pages 2-32.

[2] P. Peerani, M. Swinhoe: “Results of the ESARDA Multiplicity Benchmark Exercise”, Proc. of the 47th INMM Annual Meeting, Nashville (TN), 17-20 July 2006.

[3] P. Baeten, M. Bruggeman, P. Chard, S. Croft, D. Parker, C. Zimmerman, M. Looman, S. Guardini: “Results of the ESARDA REALS Prediction Benchmark Exercise”, ESARDA Bulletin, Nr. 31, April 2002, pages 18-22.

[4] http://gno.cesigma.free.fr/Gb/Accueil/Sommaire.htm

[5] http://www.canberra.com/pdf/Products/Systems_pdf/jcc_51.pdf

[6] N. Ensslin et al.: “Application Guide to Neutron Multiplicity Counting”, LA-13422-M (November 1998).

Table 1: Results from (zero dead-time) simulations and comparison with theoretical (point model) values.

	Counting time	Singles rate	S abs. unc.	Doubles rate	D abs. unc.	Triples rate	T abs. unc.
Case 1: Cf low intensity							
Point model		***1170***		***380.28***		***68.84***	
Experimental (DT corrected)		***1211***		***382.64***		***67.66***	
Chalmers Univ.	1000	1175	3.85	386.56	4.25	71.66	3.25
IPPE	1000	1147	2.12	362.00	1.34	61.01	0.43
JRC	52000	1167	0.21	376.61	0.13	73.70	0.88
IRSN (MCNPX direct)		1167	0.47	374.68	0.37	67.34	0.19
IRSN (MCNPX + TRIDEN)	1000	1165	2.20	374.29	1.37	67.69	0.91
Univ. Michigan		1160		376.91		73.64	
LANL		1160	0.46	372.48	0.45	66.85	0.21
Relative standard deviation		0.01		0.02		0.07	
Case 2: Cf high intensity							
Point model		***153837***		***50011***		***9053***	
Experimental (DT corrected)		***153768***		***48545***		***8347***	
Chalmers Univ.	1000	154692	23.88	51032	238.47	9432	585.63
IPPE	1000	150770	17.83	47602	82.24	8022	219.28
JRC	402	153070	25.73	48880	123.23	8760	363.82
IRSN (MCNPX direct)		153318	61.33	49240	49.24	8850	24.78
IRSN (MCNPX + TRIDEN)	1000	153282	11.80	49318	49.07	8434	72.57
Univ. Michigan		153572		49786		8656	
LANL		151826	60.73	48738	58.49	8747	27.99
Relative standard deviation		0.01		0.02		0.05	
Case 3: Pu metal							
Point model		***724***		***142.38***		***16.72***	
Experimental (DT corrected)		***721***		***129.25***		***14.29***	
Chalmers Univ.	1000	713	3.06	139.48	1.59	16.45	0.89
IPPE	1000	716	0.91	138.65	0.85	15.35	0.22
JRC	52000	722	0.17	142.17	0.74	18.31	0.41
IRSN (MCNPX direct)		701	0.14	130.46	0.09	14.24	0.03
IRSN (MCNPX + TRIDEN)	1000	700	1.51	129.97	0.51	13.93	0.23
Univ. Michigan		708		136.13		16.89	
LANL		693	0.03	130.64	0.01	14.76	0.01
Relative standard deviation		0.01		0.04		0.10	
Case 4: Pu oxide small mass							
Point model		***7297***		***904.87***		***107.36***	
Experimental (DT corrected)		***7328***		***919.14***		***113.83***	
Chalmers Univ.	1000	6534	5.87	866.51	12.48	109.03	7.85
IPPE	1000	7317	2.83	944.07	4.10	113.96	3.08
JRC	6378	7282	1.40	945.02	1.39	126.93	1.14
IRSN (MCNPX direct)		7031	6.24	892.64	1.38	110.14	0.62
IRSN (MCNPX + TRIDEN)	1000	7072	3.42	912.41	3.65	112.86	2.22
Univ. Michigan		7196		942.05		136.16	
LANL		6962	0.92	901.04	0.61	111.58	0.26
Relative standard deviation		0.04		0.03		0.09	

Table 1: Results from (zero dead-time) simulations and comparison with theoretical (point model) values.

	Counting time	Singles rate	S abs. unc.	Doubles rate	D abs. unc.	Triples rate	T abs. unc.
Case 5: Pu oxide large mass							
Point model		***147656***		***23009***		***4224***	
Experimental (DT corrected)		***146568***		***23316***		***4595***	
Chalmers Univ.	1000	130564	33.01	20957	238.98	4093	546.71
IPPE	1000	146530	16.00	22487	71.05	3814	170.95
JRC	242	147060	31.30	23456	147.31	4802	363.75
IRSN (MCNPX direct)		146731	28.43	23748	17.39	4474	11.60
IRSN (MCNPX + TRIDEN)	1000	146818	4.38	23650	24.25	3765	36.59
Univ. Michigan		144804		22940		5137	
LANL		139974	15.10	21894	17.70	3980	8.90
Relative standard deviation		0.04		0.05		0.12	
Case 6: MOX sample							
Point model		***26157***		***3411***		***371.56***	
Experimental (DT corrected)		***27772***		***3128***		***348.26***	
Chalmers Univ.	1000	25719	10.93	3397	37.14	373.18	30.04
IPPE	1000	25504	4.00	3184	10.74	303.24	17.94
JRC	2388	26135	4.60	3414	8.53	397.14	8.44
IRSN (MCNPX direct)		24784	4.63	3109	1.87	329.09	0.72
IRSN (MCNPX + TRIDEN)	1000	24773	3.95	3124	7.59	348.58	13.53
Univ. Michigan		21552		3123		349.58	
LANL		23507	2.50	2991	2.40	336.21	0.80
Relative standard deviation		0.06		0.05		0.09	

Table 2: Comparison of measurements and simulations with dead-time effects.

	Singles rate	Doubles rate	Triples rate
Case 1: Cf low intensity			
measured	**1208.08**	**380.73**	**66.62**
MCNP-PTA	1164.60	374.73	71.96
(C-E)/E	*-3.6%*	*-1.6%*	*8.0%*
MCNP-Polimi	1157.74	375.63	72.60
(C-E)/E	*-4.2%*	*-1.3%*	*9.0%*
MCNPX + post-processor	1162.61	372.82	66.65
(C-E)/E	*-3.8%*	*-2.1%*	*0.0%*
Case 2: Cf high intensity			
measured	**149338**	**43374**	**3695**
MCNP-PTA	148660	43673	3743
(C-E)/E	*-0.5%*	*0.7%*	*1.3%*
MCNP-Polimi	149976	45438	4550
(C-E)/E	*0.4%*	*4.8%*	*23.1%*
MCNPX + post-processor	149145	44398	3734
(C-E)/E	*-0.1%*	*2.4%*	*1.0%*
Case 3: Pu metal			
measured	**720.51**	**129.09**	**14.07**
MCNP-PTA	701.41	133.32	15.07
(C-E)/E	*-2.7%*	*3.3%*	*7.1%*
MCNP-Polimi	707.63	135.83	16.65
(C-E)/E	*-1.8%*	*5.2%*	*18.4%*
MCNPX + post-processor	698.72	129.50	13.69
(C-E)/E	*-3.0%*	*0.3%*	*-2.7%*
Case 4: Pu oxide small mass			
measured	**7313.46**	**912.24**	**109.29**
MCNP-PTA	7267.50	937.93	121.09
(C-E)/E	*-0.6%*	*2.8%*	*10.8%*
MCNP-Polimi	7183.27	935.75	130.34
(C-E)/E	*-1.8%*	*2.6%*	*19.3%*
MCNPX + post-processor	7059.04	906.40	108.36
(C-E)/E	*-3.5%*	*-0.6%*	*-0.9%*
Case 5: Pu oxide large mass			
measured	**142622**	**20873**	**2519**
MCNP-PTA	143100	20998	2632
(C-E)/E	*0.3%*	*0.6%*	*4.5%*
MCNP-Polimi	141739	21156	3696
(C-E)/E	*-0.6%*	*1.4%*	*46.7%*
MCNPX + post-processor	143143	21499	2053
(C-E)/E	*0.4%*	*3.0%*	*-18.5%*
Case 6: MOX sample			
measured	**27623**	**3064**	**301.8**
MCNP-PTA	25995	3344	344.2
(C-E)/E	*-5.9%*	*9.1%*	*14.0%*
MCNP-Polimi	21471	3078	320.3
(C-E)/E	*-22.3%*	*0.5%*	*6.1%*
MCNPX + post-processor	24654	3066	303.40
(C-E)/E	*-10.7%*	*0.1%*	*0.5%*

Table 3: Comparison of dead-time correction factors.

	Singles	Doubles	Triples
Case 1: Cf low intensity			
MCNP-PTA	1.002	1.005	1.024
MCNP-Polimi	1.002	1.003	1.014
MCNPX + TRIDEN	1.002	1.004	1.016
Case 2: Cf high intensity			
MCNP-PTA	1.03	1.12	2.34
MCNP-Polimi	1.02	1.10	1.90
MCNPX + TRIDEN	1.03	1.11	2.26
Case 3: Pu metal			
MCNP-PTA	1.001	1.003	1.016
MCNP-Polimi	1.001	1.002	1.014
MCNPX + TRIDEN	1.002	1.004	1.018
Case 4: Pu oxide small mass			
MCNP-PTA	1.002	1.008	1.048
MCNP-Polimi	1.002	1.007	1.045
MCNPX + TRIDEN	1.002	1.007	1.042
Case 5: Pu oxide large mass			
MCNP-PTA	1.03	1.12	1.82
MCNP-Polimi	1.02	1.08	1.39
MCNPX + TRIDEN	1.03	1.10	1.83
Case 6: MOX			
MCNP-PTA	1.005	1.021	1.15
MCNP-Polimi	1.004	1.015	1.09
MCNPX + TRIDEN	1.005	1.019	1.15

Table 4: Results from experimental pulse train processing and comparison with multiplicity shift register measurements.

	Counting time	Singles rate	S abs. unc.	Doubles rate	D abs. unc.	Triples rate	T abs. unc.	Time
Case 1: Cf low intensity								
Measured		***1247.87***	***1.58***	***380.78***	***0.84***	***66.65***	***0.48***	
Chalmers Univ.	1053.32	1244.42	4.49	382.26	2.94	67.09	2.23	3.4
IPPE	1050.00	1244.44	1.43	381.70	0.77	66.39	0.57	1.0
CEA-DAM	1053.32	1244.34	4.49	381.88	2.43	66.72	2.99	0.5
CEA-LMN		1243.94	1.57	381.90	1.14	66.74	0.75	0.7
AREVA	1040.00	1244.30	4.37	382.07	3.87	72.52	2.74	8.2
JRC	1053.24	1244.40	4.48	381.26	2.94	66.23	2.12	2.0
JRC-2	1053.32	1244.37	4.50	381.80	2.82	66.67	1.98	2.8
IKI	954.90	1243.90	1.10	382.60	1.20	67.30	2.00	1.0
IRSN	1053.29	1244.39	1.42	381.60	0.75	66.35	1.75	5.9
CANBERRA	1053.20	1244.70	4.61	381.32	3.50	66.37	2.51	0.9
Univ. Michigan	1053.30	1244.36		381.96		72.48		
LANL	1053.25	1244.39	1.42	382.23	0.92	67.07	0.71	0.8
Rel. stand. dev.		*0.000*		*0.001*		*0.034*		
Case 2: Cf high intensity								
Measured		***149378.13***	***7.30***	***43373.58***	***33.22***	***3695.29***	***71.23***	
Chalmers Univ.	1000.39	149364.24	45.84	43522.80	178.00	3142.29	352.84	4030.0
IPPE	1000.00	149360.00	15.22	43454.00	66.91	3310.80	161.28	34.0
CEA-DAM	1000.39	149362.55	45.87	43522.68	231.62	3403.39	551.33	689.3
CEA-LMN		149364.27	16.74	43470.35	77.52	3266.27	189.99	45.3
AREVA	990.00	149364.15	43.03	43492.82	245.88	3785.99	455.87	972.1
JRC	1000.34	149364.22	45.80	43525.16	286.15	3353.66	469.35	4989.0
JRC-2	1000.38	149364.26	45.87	43513.48	251.58	3328.03	644.65	218.0
IKI	999.06	149364.00	12.00	43543.00	65.00	3334.00	646.00	17.0
IRSN	1000.38	149364.26	14.50	43470.39	64.04	3271.56	144.81	2267.9
CANBERRA	1000.30	149364.63	59.18	43532.54	244.70	3554.16	627.31	1075.0
Univ. Michigan	1000.40	149360.80		43484.06		4053.14		
LANL	1000.34	149364.21	14.49	43522.92	55.69	3145.53	112.13	113.0
Rel. stand. dev.		*0.000*		*0.001*		*0.032*		
Case 3: Pu metal								
Measured		***760.288***	***1.123***	***129.141***	***0.566***	***14.099***	***0.303***	
Chalmers Univ.	1269.51	761.16	3.34	130.84	1.68	14.16	0.68	2.5
IPPE	1270.00	761.15	1.06	130.62	0.46	13.95	0.20	0.0
CEA-DAM	1269.51	761.12	3.34	131.07	1.53	14.20	0.65	0.3
CEA-LMN		760.10	1.03	130.42	0.59	14.00	0.28	0.6
AREVA	1000.00	760.10	3.45	130.45	1.57	15.50	0.88	3.4
JRC	1269.42	761.17	3.34	130.62	1.55	14.13	0.48	2.0
JRC-2	1269.51	761.14	3.34	130.86	1.66	14.23	0.72	2.4
IKI	1108.76	760.50	0.90	130.70	0.60	14.40	0.80	1.0
IRSN	1269.48	761.15	1.06	130.68	0.44	13.98	0.19	4.3
CANBERRA	1269.40	761.33	3.09	130.63	1.52	14.16	0.62	1.1
Univ. Michigan	1269.50	761.43		130.68		15.50		
LANL	1269.41	761.16	1.06	130.84	0.53	14.16	0.22	0.8
Rel. stand. dev.		*0.001*		*0.001*		*0.009*		

Table 4: Results from experimental pulse train processing and comparison with multiplicity shift register measurements.

	Counting time	Singles rate	S abs. unc.	Doubles rate	D abs. unc.	Triples rate	T abs. unc.	Time
Case 4: Pu oxide small mass								
Measured		***7353.24***	***4.43***	***912.29***	***3.76***	***109.32***	***2.83***	
Chalmers Univ.	1070.66	7345.31	11.26	913.10	8.62	110.78	6.96	28.3
IPPE	1070.00	7345.30	3.56	906.72	3.94	106.56	2.55	3.0
CEA-DAM	1070.66	7345.18	11.26	910.12	9.43	110.11	8.22	4.1
CEA-LMN		7345.65	3.09	906.43	3.66	107.00	2.35	2.2
AREVA	1000.00	7345.65	12.16	910.25	10.89	117.06	7.27	29.9
JRC	1070.62	7345.30	11.28	908.96	9.20	108.53	6.17	37.0
JRC-2	1070.66	7345.27	11.25	906.70	6.84	109.61	7.89	11.6
IKI	1053.90	7345.40	2.60	907.40	3.30	110.00	7.70	1.0
IRSN	1070.65	7345.27	3.56	906.65	4.12	106.49	2.66	38.3
CANBERRA	1070.60	7345.47	9.24	908.95	10.54	108.76	6.44	8.0
Univ. Michigan	1070.60	7345.64		907.41		118.75		
LANL	1070.61	7345.29	3.57	913.10	2.73	110.78	2.21	3.7
Rel. stand. dev.		*0.000*		*0.003*		*0.015*		
Case 5: Pu oxide large mass								
Measured		***142661.62***	***16.19***	***20873.04***	***40.18***	***2518.91***	***175.20***	
Chalmers Univ.	1001.80	142611.58	33.83	20940.06	255.57	2459.96	702.97	3700.0
IPPE	1000.00	142610.00	10.85	20909.00	63.13	2432.50	142.18	33.0
CEA-DAM	1001.80	142609.95	33.91	20949.26	164.21	2473.05	551.68	630.0
CEA-LMN		142611.03	14.21	20913.85	63.36	2420.11	141.24	44.1
AREVA	1000.00	142611.03	33.80	20931.81	237.37	2911.00	743.75	907.5
JRC	1001.76	142611.49	34.04	20925.37	209.17	2473.20	431.78	4536.0
JRC-2	1001.79	142611.59	33.92	20973.49	108.53	2562.83	566.41	208.0
IKI	1000.84	142611.00	12.00	20987.00	56.00	2568.00	572.00	16.0
IRSN	1001.79	142611.59	10.72	20912.59	67.72	2422.62	171.51	2096.9
CANBERRA	1001.80	142612.12	38.28	20934.08	183.00	2462.23	460.18	916.4
Univ. Michigan	1001.80	141606.60		20776.55		2872.58		
LANL	1001.75	142611.47	10.76	20939.33	80.74	2458.78	223.22	104.0
Rel. stand. dev.		*0.002*		*0.002*		*0.021*		
Case 6: MOX sample								
Measured		***27662.76***	***5.23***	***3063.97***	***15.55***	***301.84***	***19.31***	
Chalmers Univ.	1018.88	27658.27	17.35	3082.96	35.38	292.67	47.84	200.0
IPPE	1020.00	27658.00	5.50	3053.40	9.83	276.40	10.37	6.0
CEA-DAM	1018.88	27657.91	17.33	3059.32	18.40	303.23	40.18	31.3
CEA-LMN		27658.42	6.25	3053.55	11.82	274.67	11.99	7.8
AREVA	1000.00	27658.43	18.47	3073.31	35.94	310.16	44.15	118.4
JRC	1018.84	27658.23	17.33	3075.91	26.28	283.85	36.96	224.0
JRC-2	1018.87	27658.24	17.33	3071.09	22.21	294.35	38.00	40.0
IKI	912.89	27661.30	5.50	3071.90	10.60	281.50	37.40	3.0
IRSN	1018.87	27658.24	5.48	3052.45	9.93	276.79	10.75	179.2
CANBERRA	1018.80	27658.48	21.07	3075.86	35.71	283.15	35.56	52.1
Univ. Michigan	1018.90	27657.43		3055.31		315.23		
LANL	1018.84	27658.22	5.48	3082.92	11.18	292.69	15.15	14.2
Rel. stand. dev.		*0.000*		*0.004*		*0.031*		

Table 5: Contributors to the "ESARDA Multiplicity Benchmark Exercise".

Participant	Contributors	Institution
JRC	Paolo Peerani Z. Dzbikowicz M. Marin Ferrer Luc Dechamp Pascal Dransart	European Commission, Joint Research Centre, IPSC, Ispra, Italy
LANL	Martyn Swinhoe Steve Tobin	N-1, Safeguards Science and Technology Group Los Alamos (NM), USA
CANBERRA (Univ.Birmingham)	Stephen Croft Louise G. Evans	CANBERRA Industries Inc Meriden (CT), USA
IPPE	Boris Ryazanov Vladimir Nyzhnik Valery Boulanenko	Institute for Physics and Power Engineering, RMTC, Obninsk, Russia
IRSN	Anne-Laure Weber Thierry Lambert	Institut de Radioprotection et Sûreté Nucléaire, IRSN/DSMR/SATE, Fontenay-aux-Roses, France
CEA-DAM	Raphael Oddou	Commissariat a l'Energie Atomique, CEA/DAM, Bruyères-le-Châtel, France
CEA-LMN	Anne-Cecile Raoux	Commissariat à l'Energie Atomique, DTN/SMTM/LMN, Cadarache, France
Chalmers University	Berit Dahl Imre Pazsit	Dept. of Nuclear Engineering, Chalmers University of Technology, Goteborg, Sweden
IKI	Janos Bagi Jozsef Huszti	Institute of Isotopes of the Hungarian Academy of Sciences Budapest, Hungary
AREVA	Lionel Tondut	AREVA NC, établissement de La Hague, Baumont Hague, France
Univ. Michigan	Sara Pozzi Shaun Clarke Eric Miller	University of Michigan, Dept. Nucl. Eng., Ann Arbor (MI), USA

Figures 2a, 2b, 2c, 2d, 2e, 2f: Plots of ratios of computed values (full simulations - phase 3) versus predicted values from point model.

Figure 2a

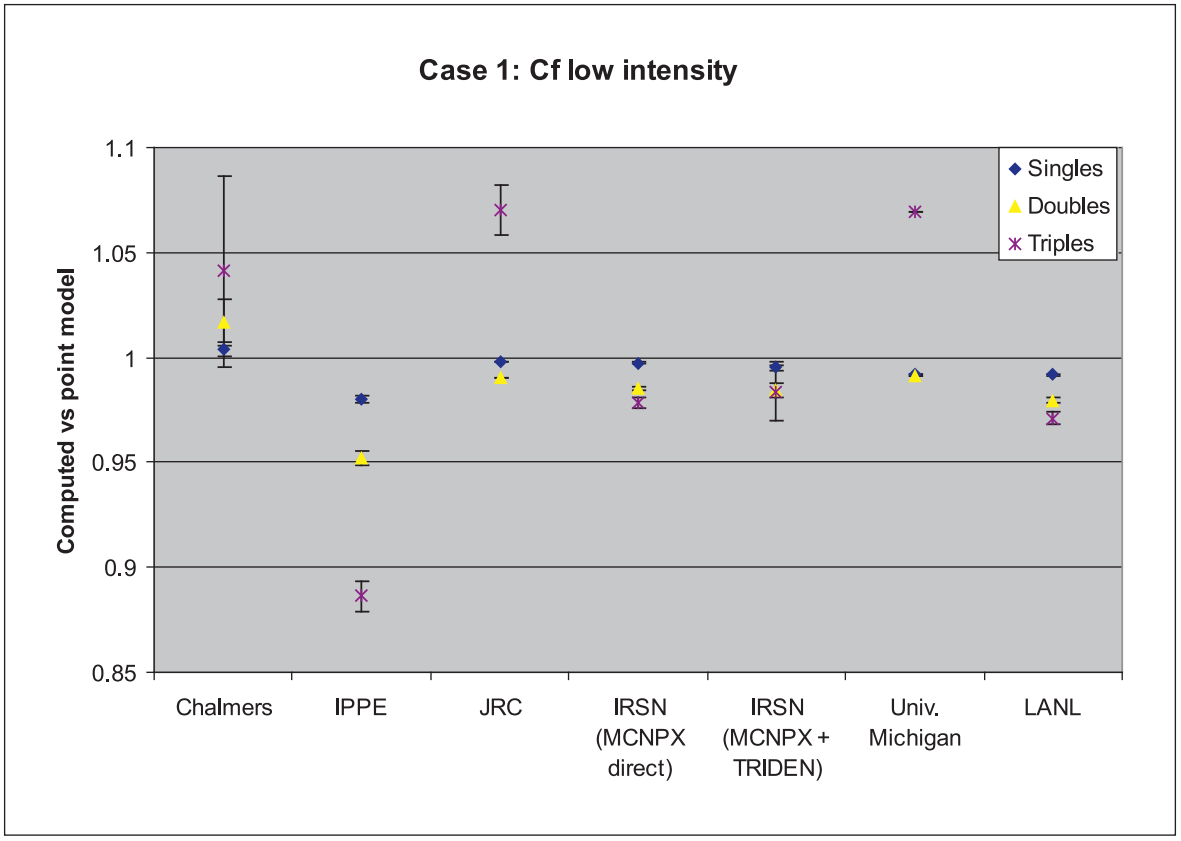
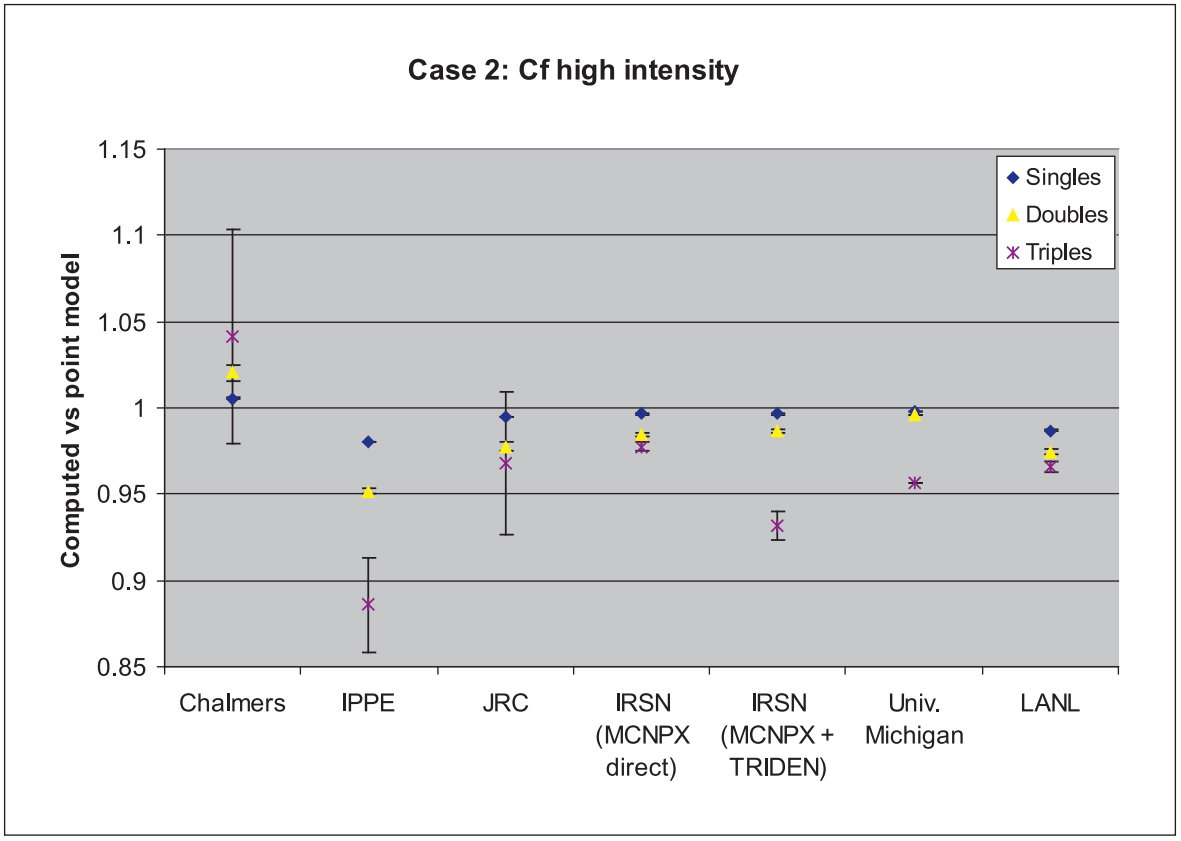


Figure 2b



Figures 2a, 2b, 2c, 2d, 2e, 2f: Plots of ratios of computed values (full simulations - phase 3) versus predicted values from point model.

Figure 2c

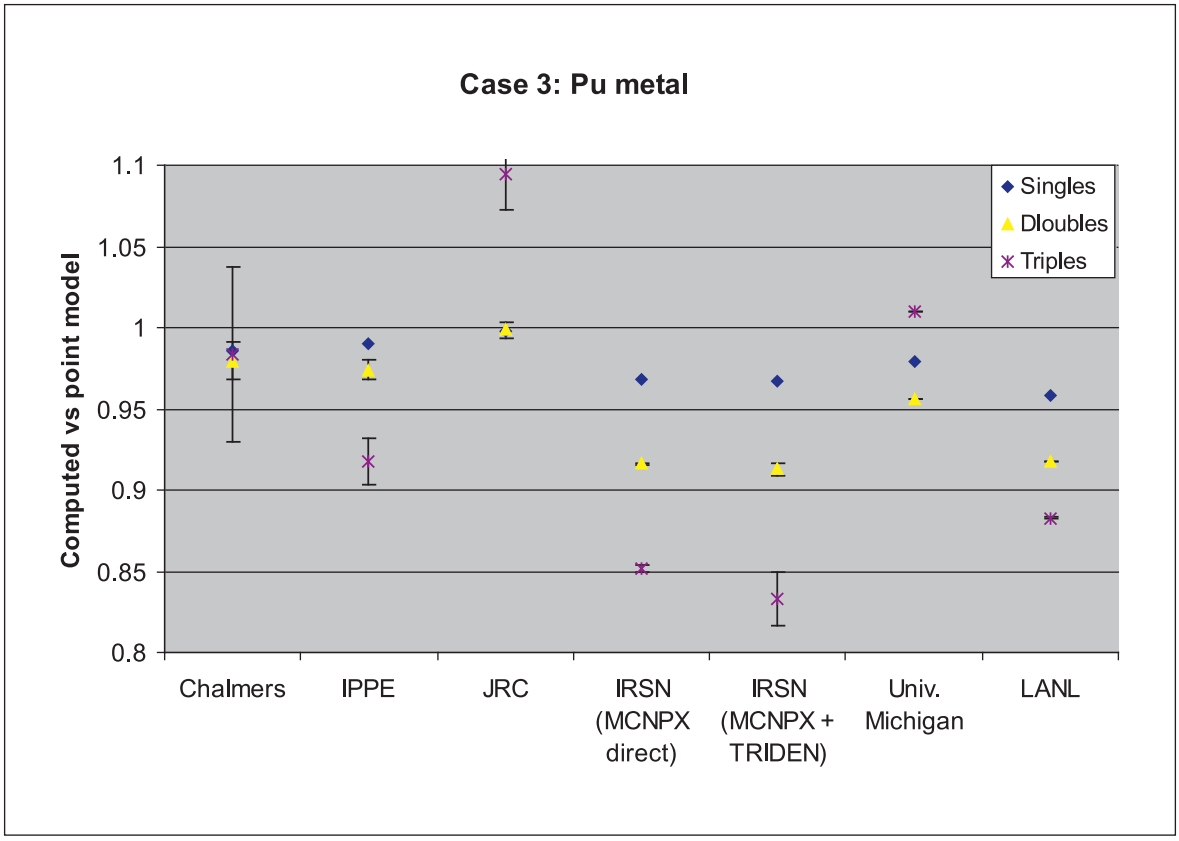
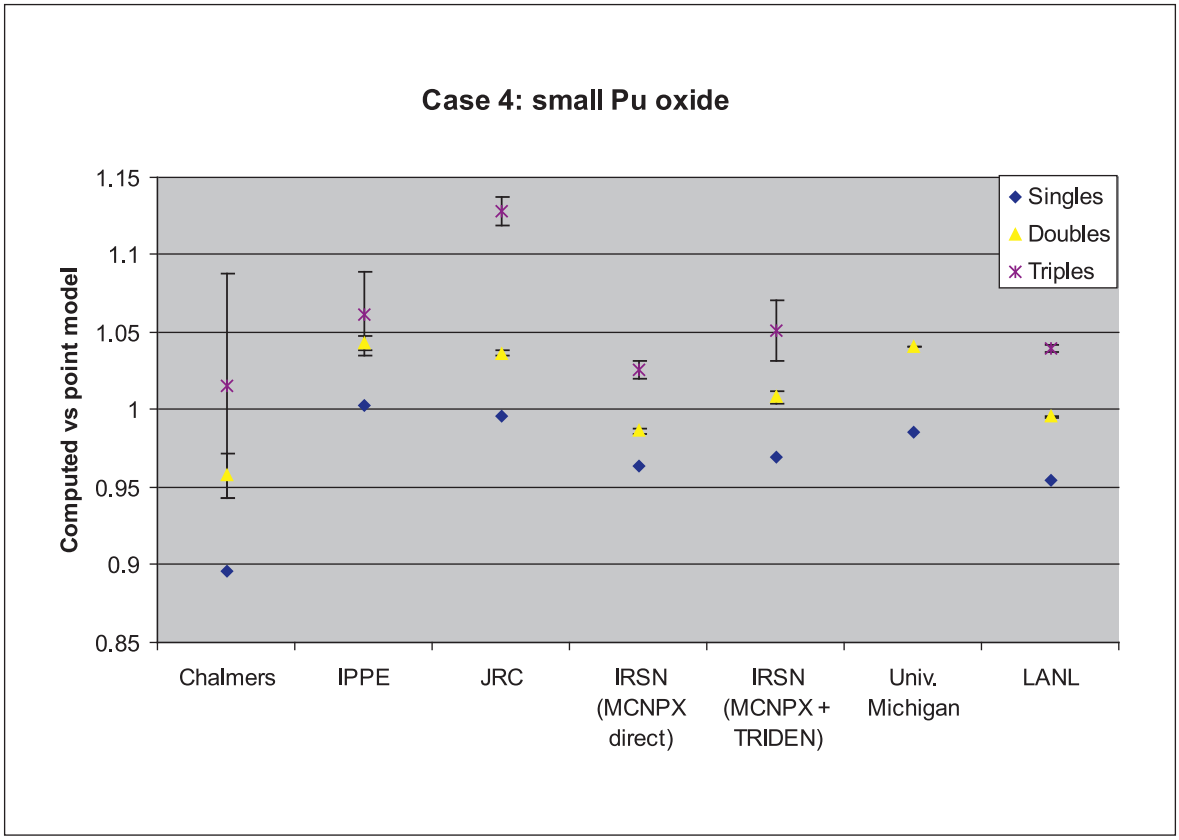


Figure 2d



Figures 2a, 2b, 2c, 2d, 2e, 2f: Plots of ratios of computed values (full simulations - phase 3) versus predicted values from point model.

Figure 2e

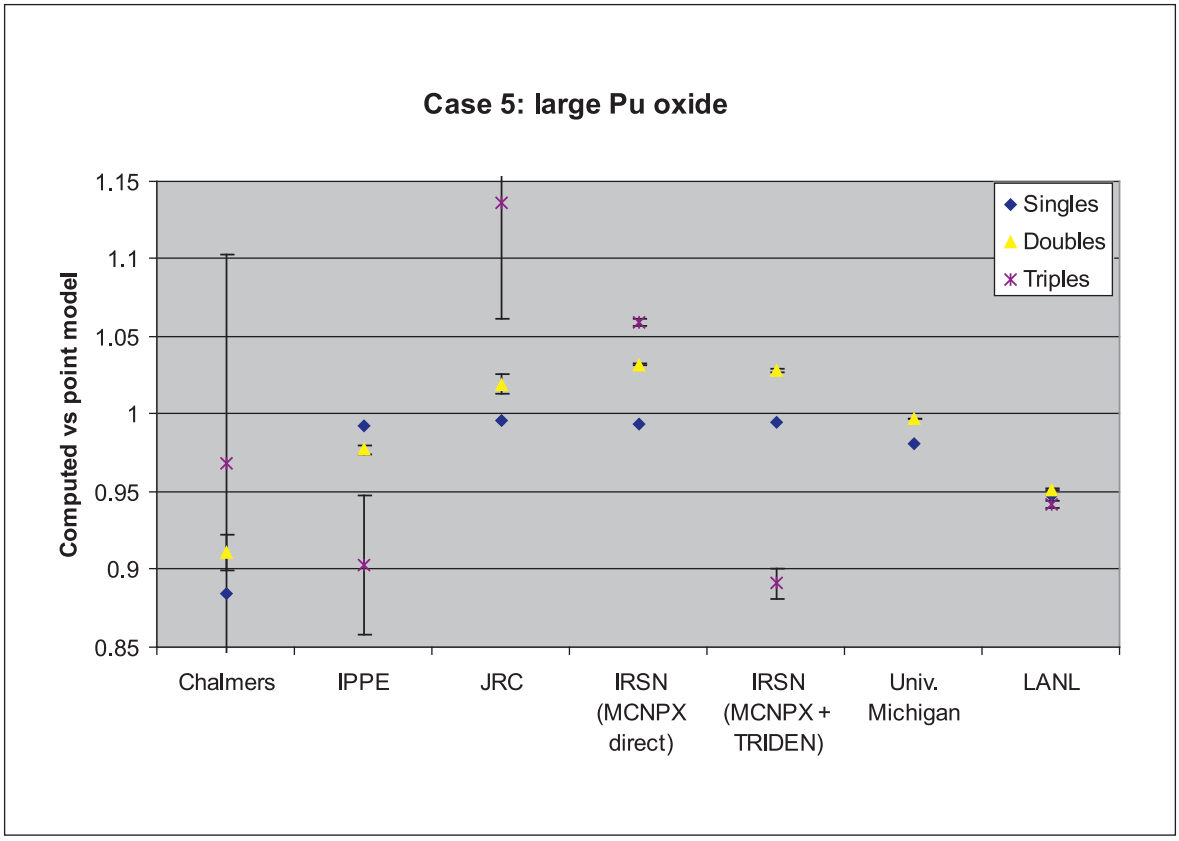
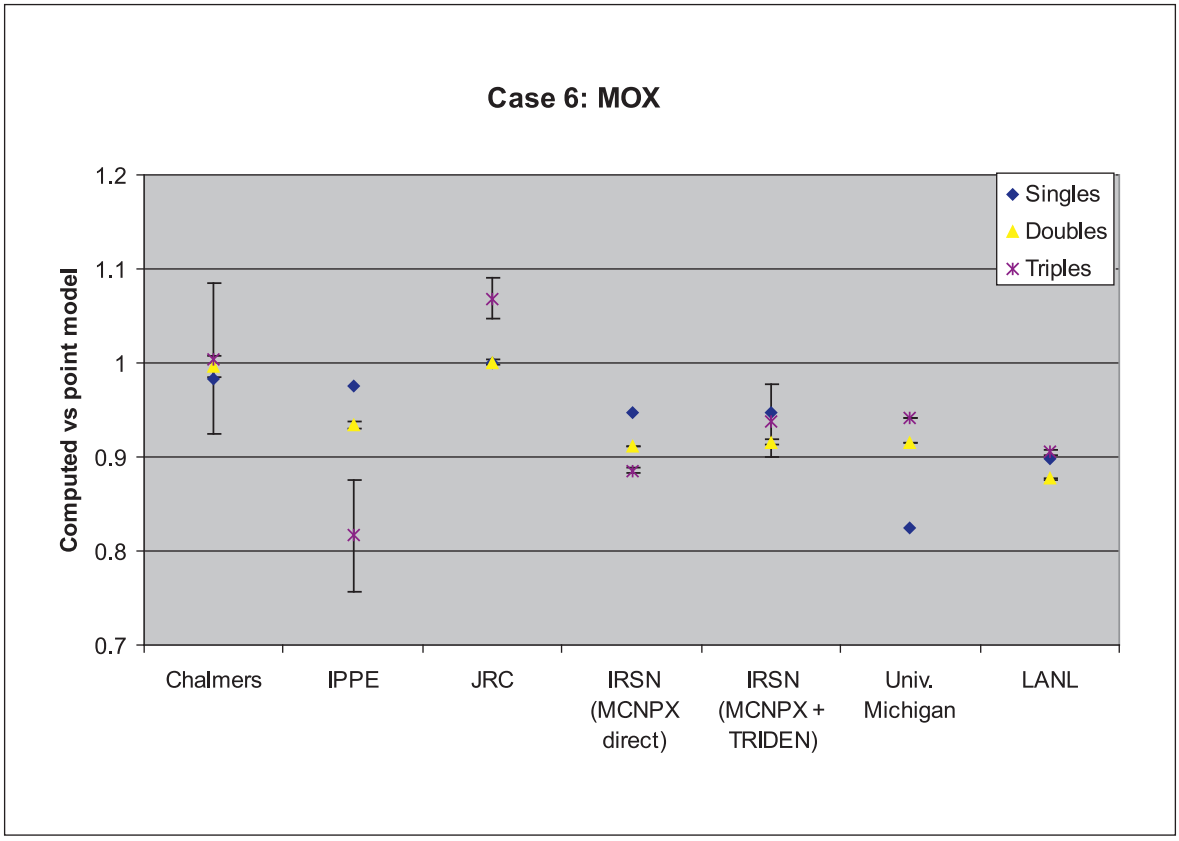


Figure 2f



Figures 3a, 3b, 3c, 3d, 3e, 3f: Plots of ratios of computed values (pulse train analysis - phase 4) versus measured values from Multiplicity Shift Register.

Figure 3a

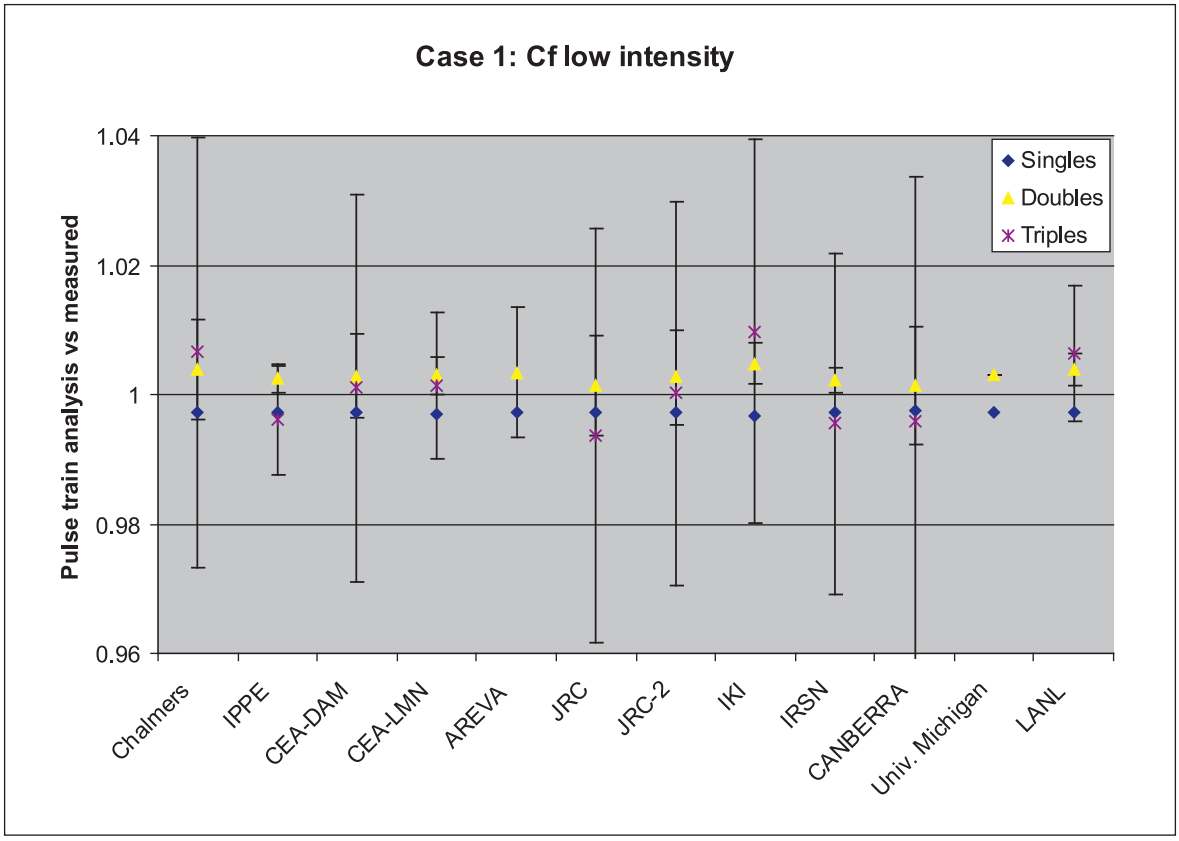
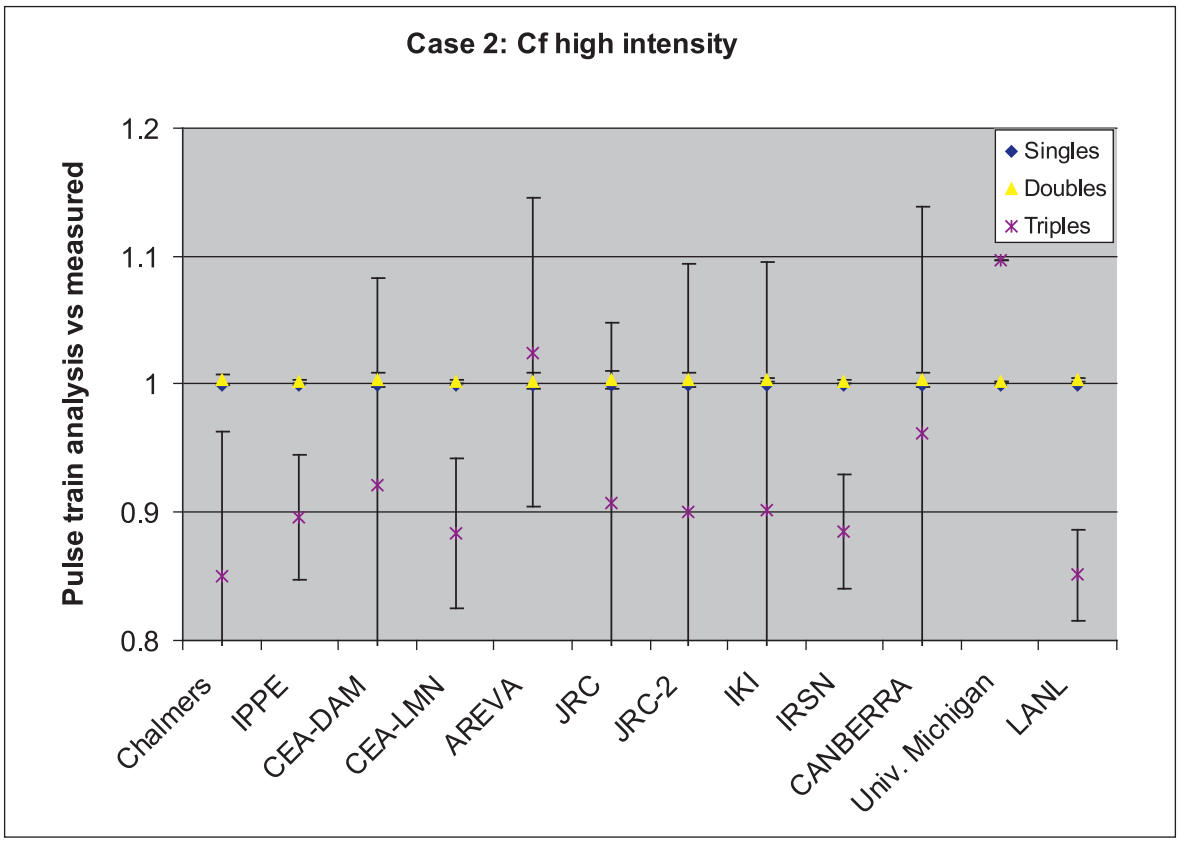


Figure 3b



Figures 3a, 3b, 3c, 3d, 3e, 3f: Plots of ratios of computed values (pulse train analysis - phase 4) versus measured values from Multiplicity Shift Register.

Figure 3c

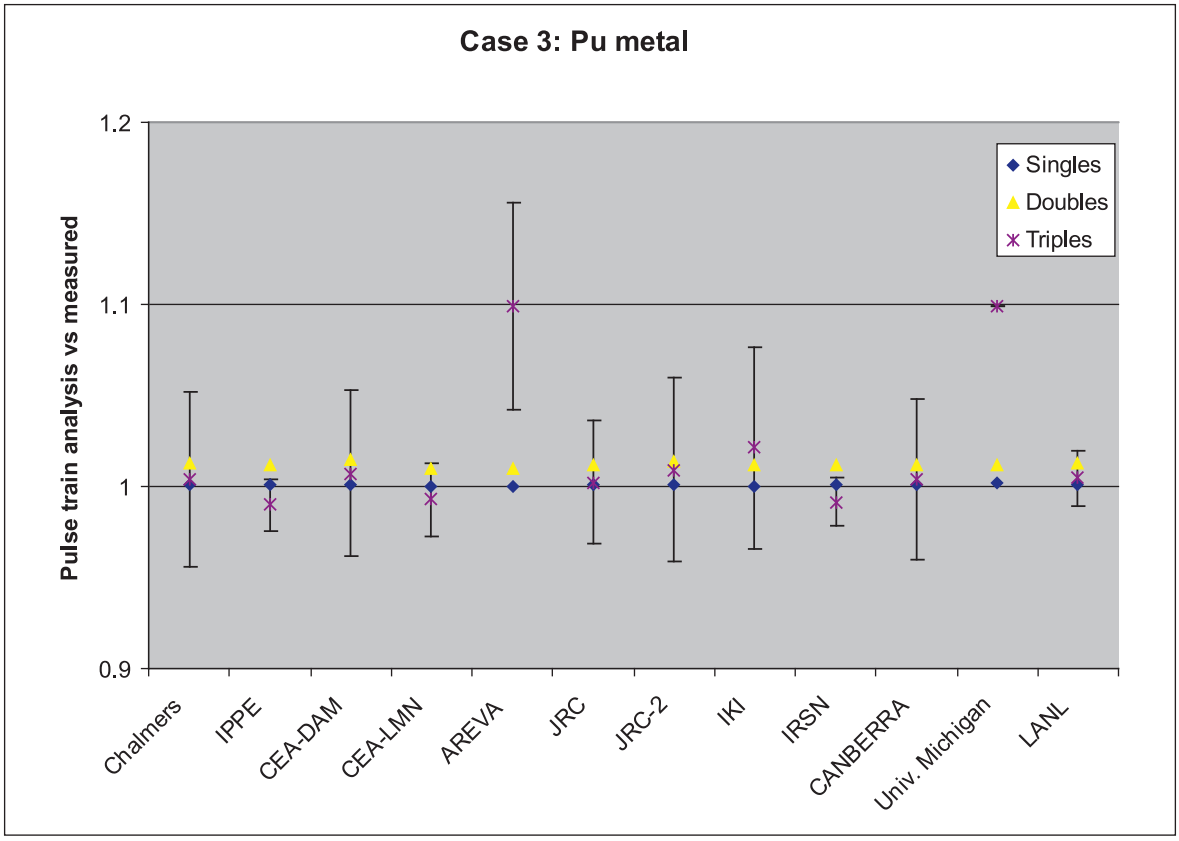
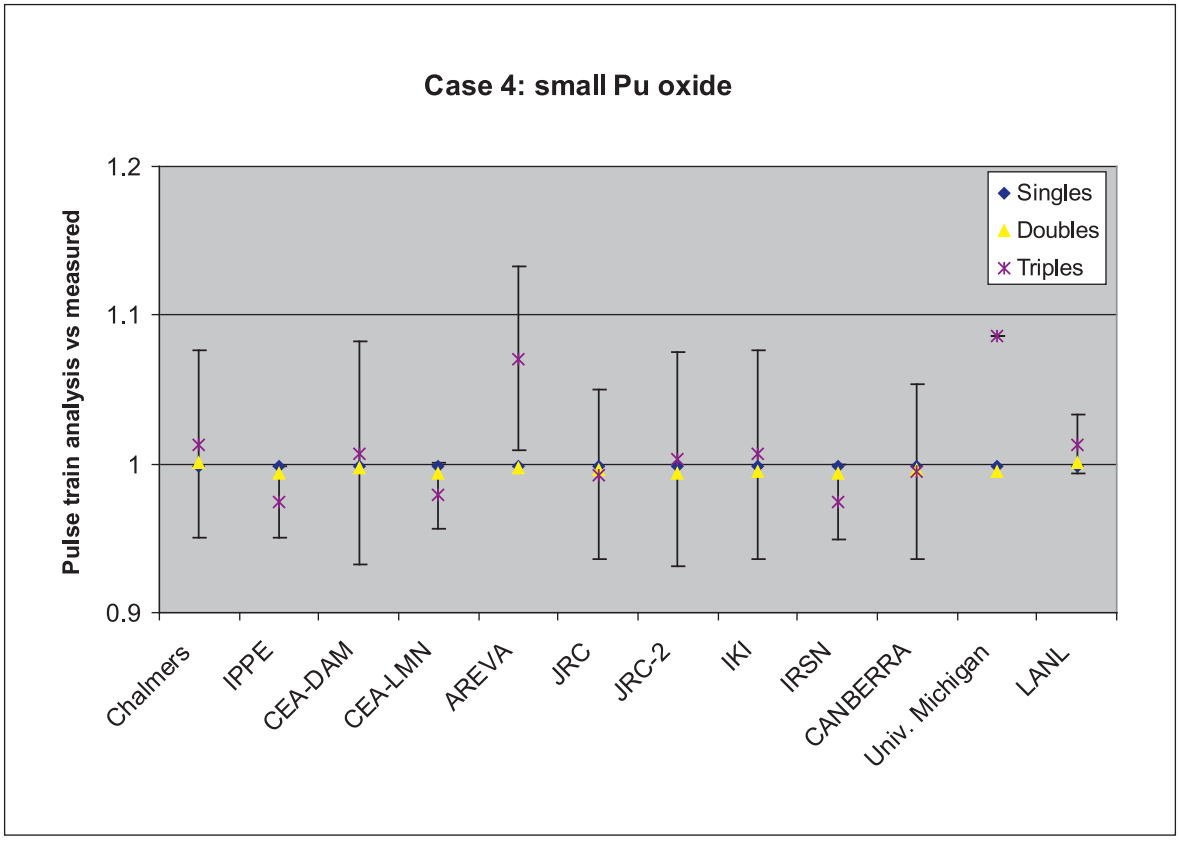


Figure 3d



Figures 3a, 3b, 3c, 3d, 3e, 3f: Plots of ratios of computed values (pulse train analysis - phase 4) versus measured values from Multiplicity Shift Register.

Figure 3e

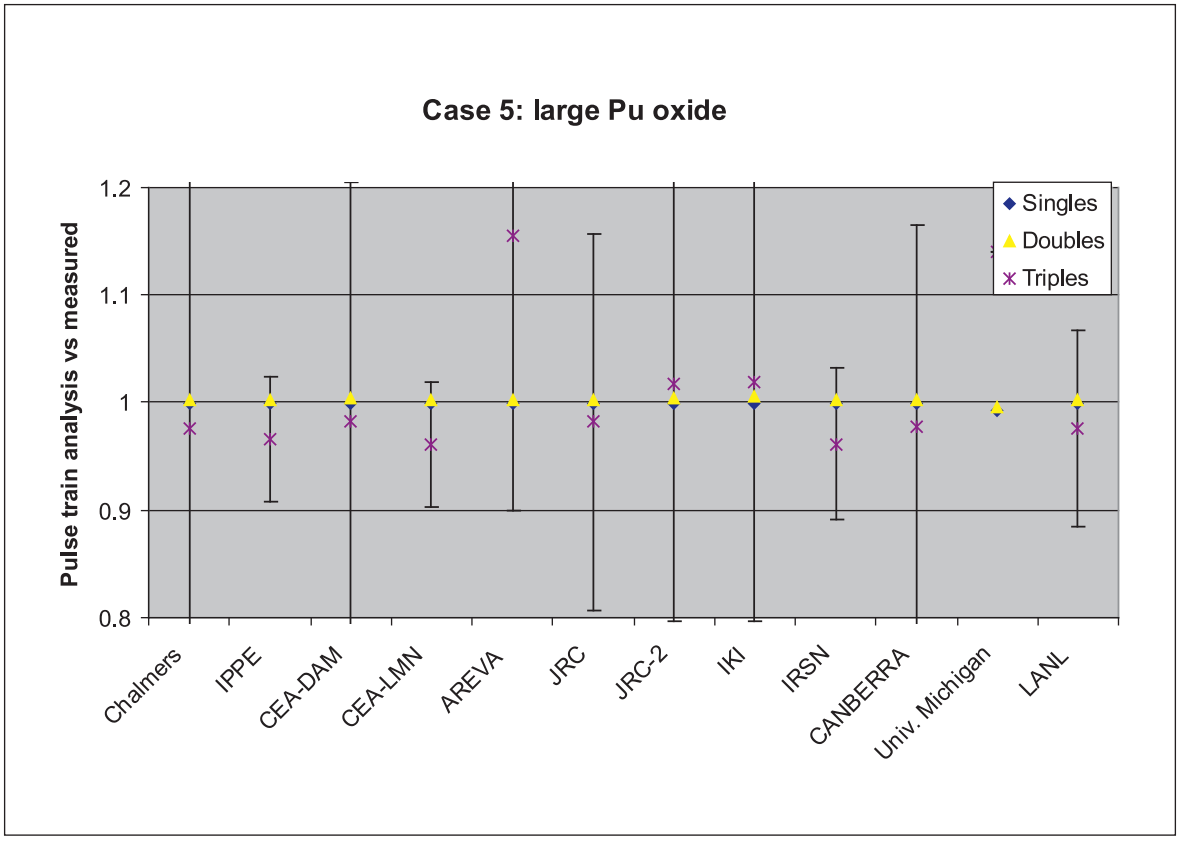


Figure 3f

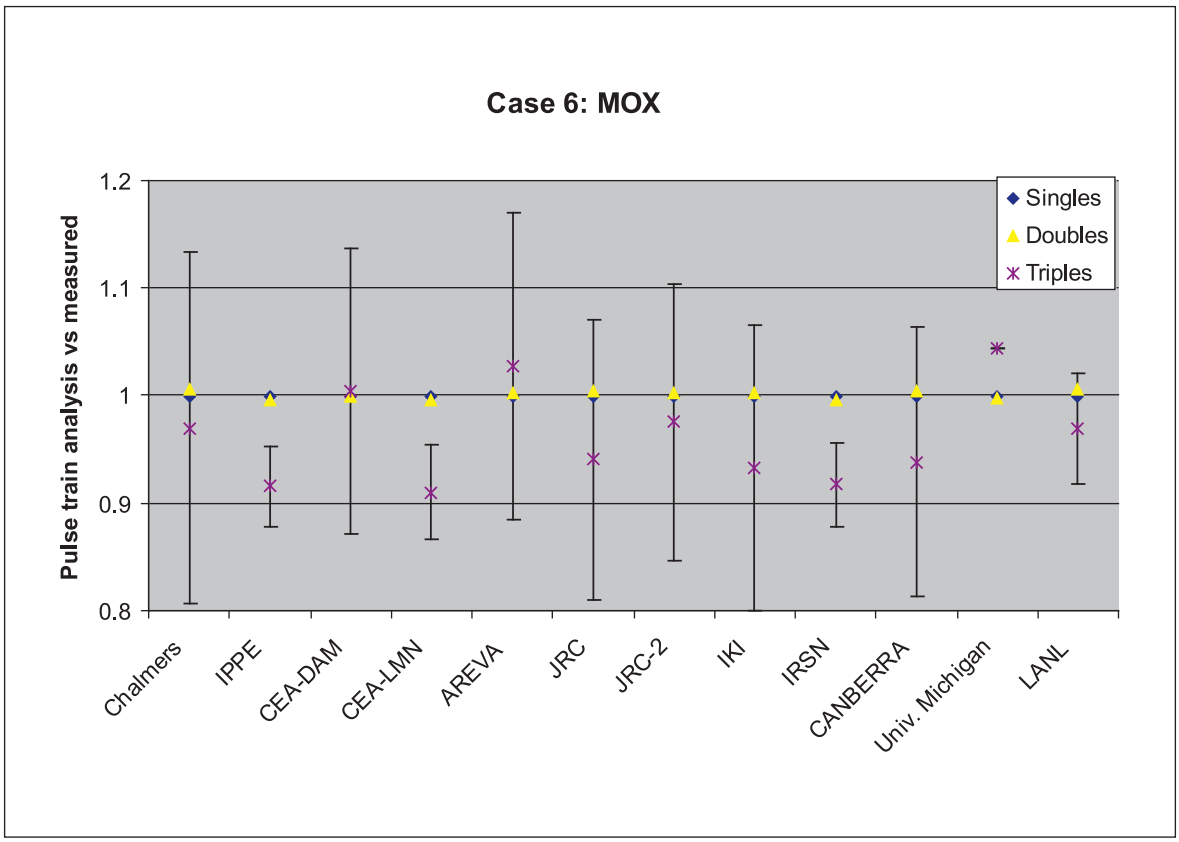


Figure 4: S, D and T plotted in ascending order for trend analysis.

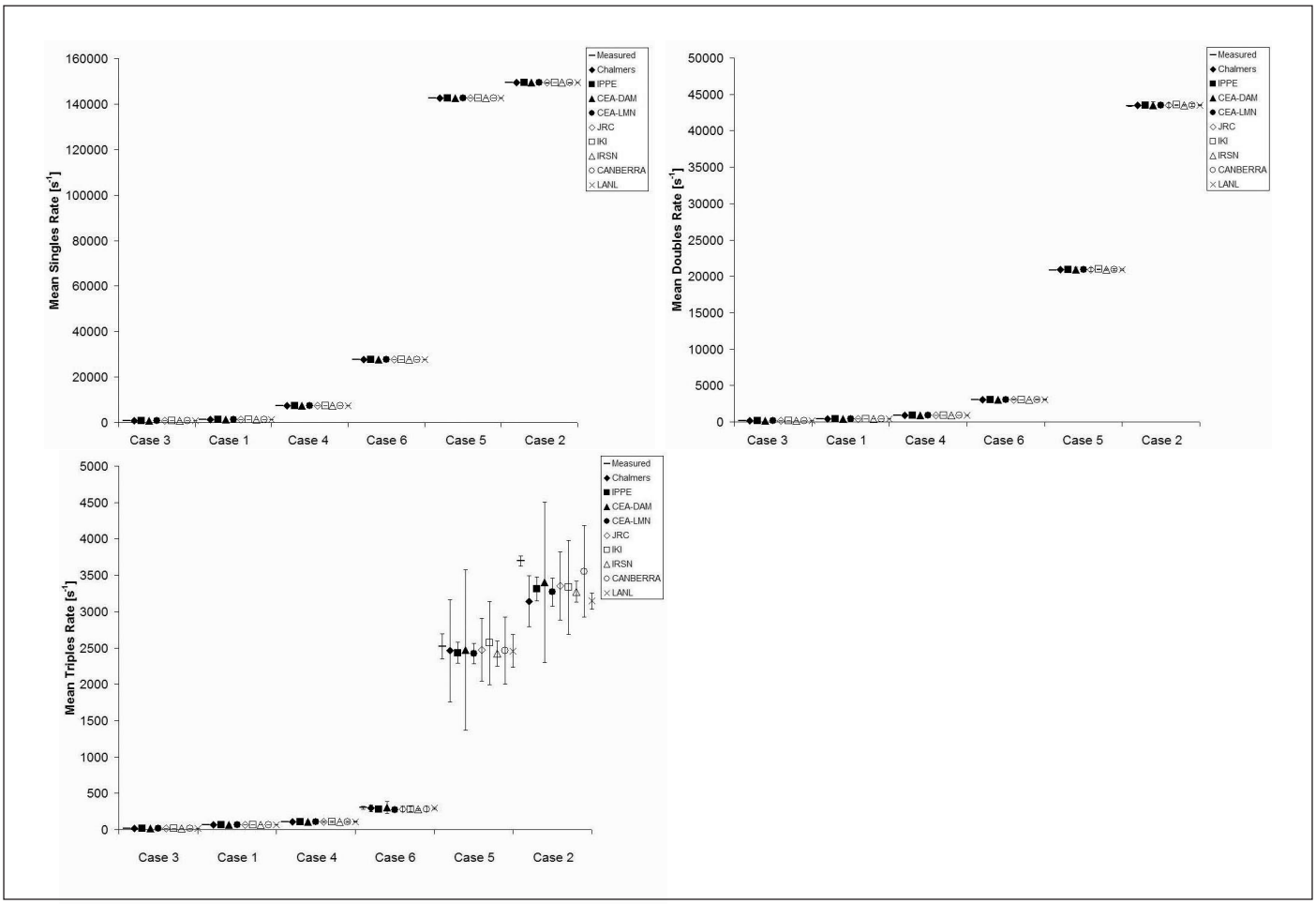


Figure 5a: Measured and calculated mean Singles count rates for each case, together with reported uncertainties.

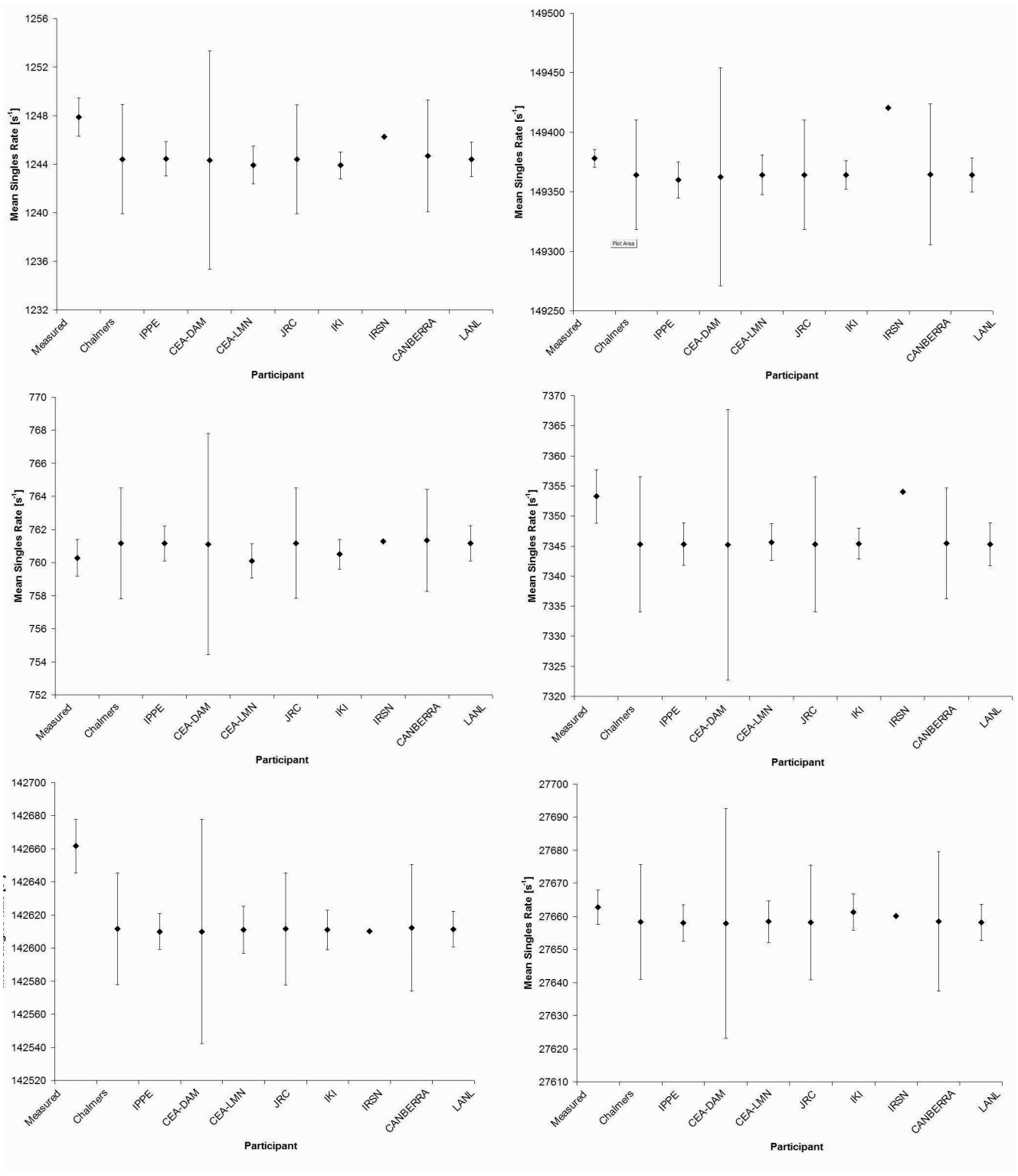


Figure 5b: Measured and calculated mean Doubles count rates for each case, together with reported uncertainties.

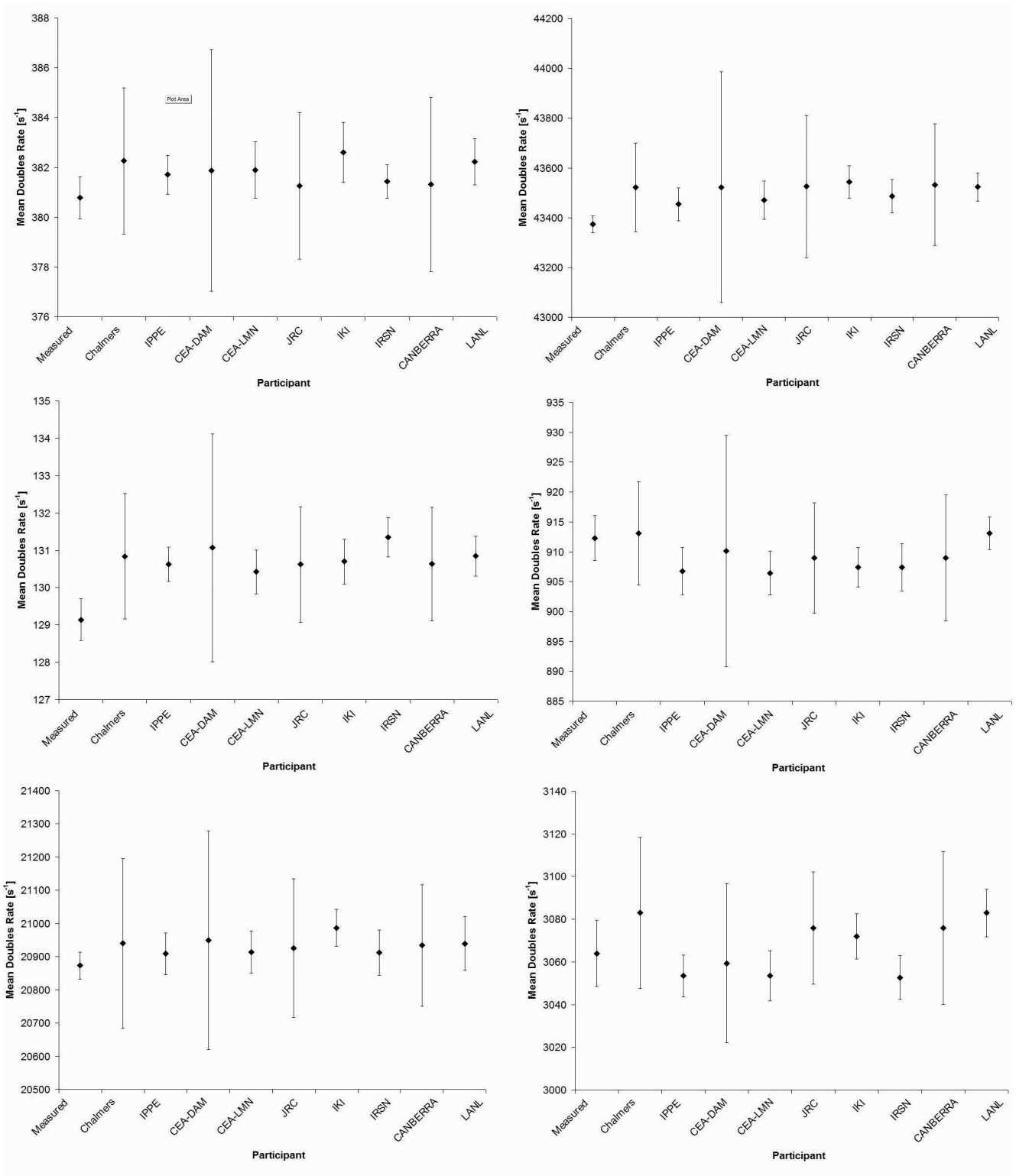
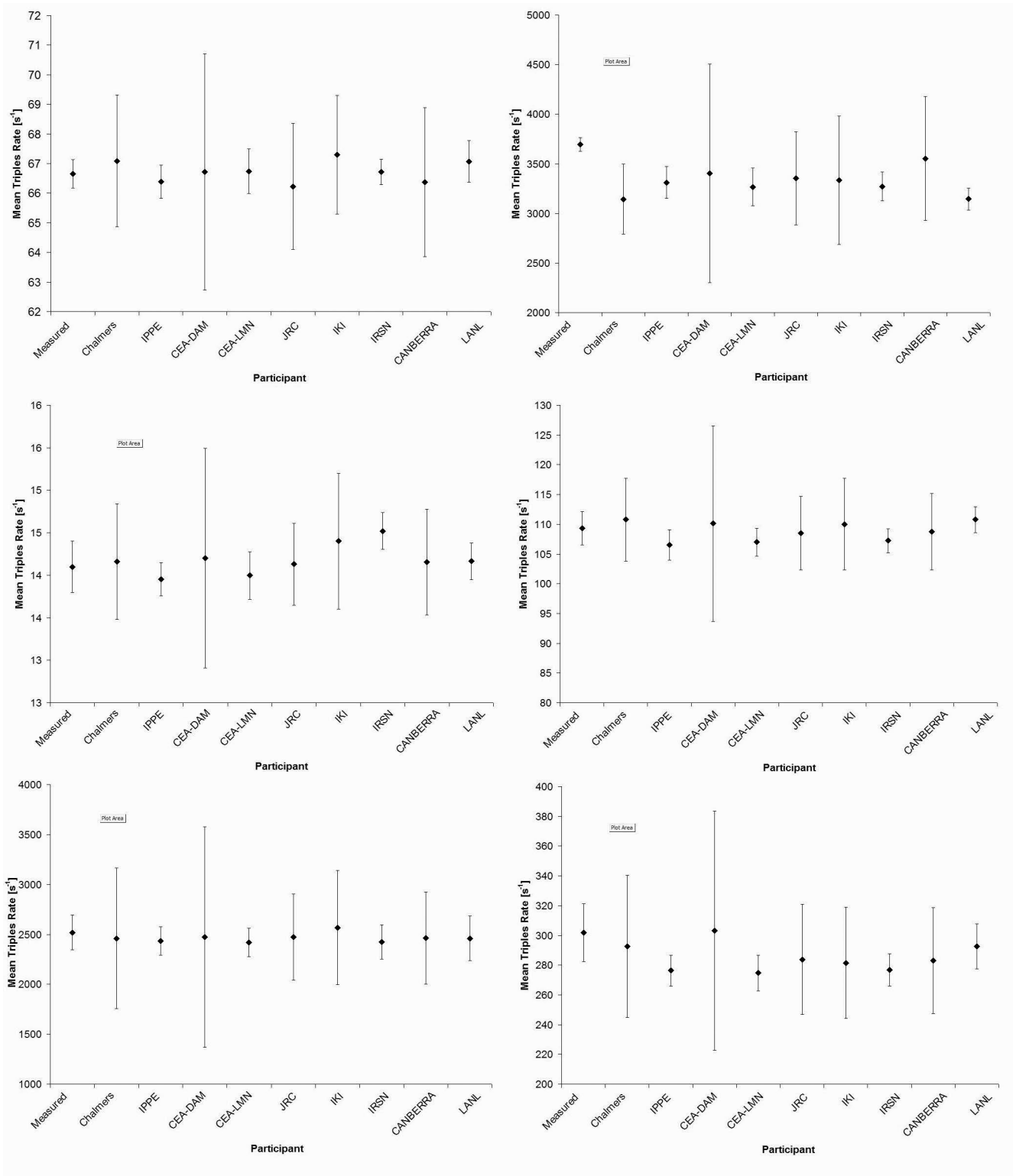


Figure 5c: Measured and calculated mean Triples count rates for each case, together with reported uncertainties.



A Good Practice Guide for the use of Modelling Codes in Non Destructive Assay of Nuclear Materials

Editor: **P.M.J. Chard**[1]

List of principal contributors from the ESARDA NDA Working Group:
P. M. J. Chard[1], **S. Croft**[2], **M.Looman**[3], **P. Peerani**[4], **H. Tagziria**[4], **M. Bruggeman**[5], **A. Laure-Weber**[6]
1. CANBERRA UK Ltd
2. CANBERRA Industries
3. Consulenze Tecniche, Italy
4. European Commission, Joint Research Centre
5. SCK / CEN
6. IRSN / Fontenay

Executive Summary

The IAEA has requested that the accepted principles of best practice for the use of radiometric modelling codes, in the Non Destructive Assay (NDA) field of the nuclear industry, should be documented. These include various code types, from discrete ordinate and Monte Carlo transport codes, to reactor physics "burnup codes". In the nuclear industry, these codes are used for a variety of application domains including nuclear material safeguards, to waste assay and environmental remediation.

The intention of this guide, by documenting best practice, is to both provide confidence for technical, management and regulatory staff, in the validity of the results of modelling codes, and provide a convenient knowledge base for technical staff in this highly specialist field.

A specialist group of experts was convened under the auspices of the ESARDA NDA working group, seeking specialist input from recognized experts in the industry as appropriate.

The resulting "good practice guide" is not intended as an exhaustive, prescriptive document. Rather, it is hoped that practitioners, managers and regulators, can use the document to provide guidance as to acceptable practices governing the use of these specialist codes. It should be noted that some degree of prior familiarity with the physics, codes, modelling techniques and applications is assumed; the guide is not suitable for a complete novice.

Following introductory remarks, scope and overview of modelling methods the bulk of the guide is contained in 7 targeted sections. These set out good practice associated with key aspects which are:

- *Problem definition,*
- *Benchmarking / validation,*
- *Training / competency,*
- *Quality Assurance,*
- *Nuclear Data,*
- *Physics treatments,*
- *Uncertainties.*

A reference list is provided allowing the reader to explore specific aspects in detail. For ease of reference an Appendix summarising important basic nuclear data is provided.

It is concluded that modelling tools are well developed and in widespread use and, properly applied are powerful and accurate. It is anticipated that the state of best practice will continue to evolve.

1. Introduction

Computer modelling codes are widely used as design tools for Non Destructive Assay (NDA) equipment, to assess performance and to predict the effects under extremes of conditions. Modelling codes have the distinct advantage over experimental techniques, in that complex geometries may be easily represented, without the need for radionuclide / fissile standards. Moreover, it is possible to model geometric conditions for which it is impossible or highly impractical to take measurements under controlled conditions. There are a variety of codes used, including both Monte Carlo based codes such as MCNP™ (and variants) and MCBEND, and analytical codes such as ANISN and ISOCS.

The increasing availability of powerful computer processors, combined with the ease of graphic visualisation, means that the fields of applicability of computer modelling techniques in NDA, are broadening. Whilst historically, modelling techniques were a valuable design aid, being used by NDA engineers and physicists to determine optimum NDA system designs, reliance was still placed upon experimental calibration using validated, representative samples and radionuclide / fissile standards. Especially in the field of nuclear materials safeguards, confidence in the validity of the calibrations is vital. However, the increasing sophistication of computer modelling codes and

techniques, combined with the reduction in availability of nuclear material standards, is now leading to the use of computer modelling to perform direct "source-less" calibrations in an absolute sense.

Modelling, by definition, mimics a real process using a mathematical representation of a physical system. It is therefore not perfect and is limited by the validity of the assumptions and the appropriateness of the model employed. Limitations exist as a result of a number of factors. These include the validity of the geometry model, the accuracy of the nuclear data employed by the code, and the validity of the physics treatments and any interpretational models used by the software, to convert the raw reaction rates, into a representation of the instrument response.

The increasing use of modelling codes is leading to a higher profile for these techniques in the nuclear industry. When one considers that modelling is now used for direct calibrations of NDA systems, it should not be a surprise that the industry is coming under increasing scrutiny by regulatory authorities and senior managers within the nuclear industry. There are legitimate concerns as to how confidence can be assured, in the accuracy of the results of NDA systems for which modelling has played an important role in determining the system configuration / calibration. The fact that this is a highly specialised industry, and that the use of modelling codes requires a high level of expertise by their practitioners, can lead to a "black art" perception, which can only accentuate these concerns. Confidence in the results of modelling codes can only result from the rigorous adoption of a number of "best practice" guidelines by the modelling practitioners, comprising both technical and non-technical considerations. Technical considerations include the nuclear data used, the validity of the physics treatments and interpretational models, benchmarking the code under representative conditions, and the use of specific codes according to recognised procedures. Non-technical factors include Quality Assurance, training and competency of the modelling practitioner.

It is recognised that there are a large number of codes in use, including application-specific vari-ants of established codes written by a different organisation from the code originator. It would be impractical to develop a generic best practice document, including specific information for individual codes. The scope of this document is therefore not limited to any specific modelling codes. However, the particular families of codes for which the document applies, is described, the generic best practice principles being valid across this full range of code types. It is also recognised that codes are constantly being developed and new fields of application identified. Their use for Research and Development including design of specialist NDA equipment, has clear long term benefits for the nuclear industry, for which it would be of no benefit to impose limitations on their conditions of use. The use of modelling codes for specialist / design applications, is therefore considered to be outside of the scope of this document. This document applies to the use of codes for functions which have a direct impact on the results produced by an NDA system, including such activities as calibration. Some of the best practice principles, are equally valid for design and R&D, but their relevance in these areas should be considered according to the specific application.

In the field of radiometric measurements, various standards and "good practice guides" exist, see for example the UK standard guide [1]. However, in the expanding field of computer modelling, such standards do not exist.

This guide addresses the above concerns, describing recognised industry best practice techniques for the application of computer modelling tools in NDA. The document has been produced under the auspices of the ESARDA NDA working group, by a group of specialists from both ESARDA organisations and organisations outside of the EU. They include representatives from Nuclear Operations organisations, NDA equipment suppliers, R&D laboratories, and regulatory authorities. In preparing this document, a wealth of experience has been drawn upon, from specialists active in this field. For example, we have worked in collaboration with the IAEA, who have recently produced a guideline document to describe best practice procedures within the IAEA, based on a co-ordinated experts meeting [2]. It is hoped that these new "best practice" guidelines will be of use to the nuclear industry including managers of plant operations organisations, NDA system physicists / engineers, as well as regulatory authorities who must be satisfied in the integrity of NDA systems.

As the field evolves and methods and nuclear data improve it will be necessary to periodically revisit this guide to allow a status update on specific points, however our aim has been to assemble good practices of enduring value.

2. Scope

The intention of this guide is to document established best practice methodologies that will ensure correct use of modelling codes, as applied to the direct calibration of Non Destructive Assay (NDA) equipment. When applied to calibration of systems,

Application		Code families			
Sample type	**Application**	**Standard Monte Carlo codes (e.g. MCNP, MCBEND, TRIPOLI, GEANT)**	**Modified Monte Carlo codes (e.g. MCNP-PTA, MCNP-REN)**	**Deterministic codes (e.g. ANISN, ISOCS, MERCURAD, ISOTOPIC, TORT)**	**Reactor Physics codes (e.g. FISPIN, ORIGEN, CESAR)**
VLRM	Sentencing	√		√	
LLW	Sentencing, NMA, criticality control, process control	√	√	√	√
ILW	Sentencing, NMA, criticality control, process control	√	√		√
Fresh fuel	NMA, criticality control, process control	√	√		√
Irradiated fuel	Sentencing, NMA, criticality control, process control	√	√		√
Contaminated items	Decontamination, decommissioning operations control	√	√	√	

Table 1: Scope of codes and areas of application.

the use of the modelling codes has a direct impact on the output results, and as such, it is very important to ensure the validity of the modelling performed. A large variety of codes is in use in the NDA industry, and it is not intended for this guide to be prescriptive to individual codes. Instead, the principles documented in this guide are relevant to the full range of codes.

The particular families of codes for which this document applies, is described below, the generic best practice principles being valid across this full range of code types. It is also recognised that codes are constantly being developed and new fields of application identified. Their use for Research and Development including design of specialist NDA equipment, has clear long term benefits for the nuclear industry, for which it would be of no benefit to impose limitations on their conditions of use. The use of modelling codes for specialist / design applications, is therefore considered to be outside of the scope of this document. This document applies to the use of codes for functions which have a direct impact on the results produced by an NDA system, including such activities as calibration. Some of the best practice principles, are, of course, equally valid for design and R&D, but their relevance in these areas should be considered according to the specific application.

The range of code types includes the following:

1. Analytical codes
2. Monte Carlo transport codes.
3. Deterministic transport codes
4. Reactor physics codes

In the NDA industry, these codes are used for a wide variety of applications, indicated in Table 1. This covers all application areas, in nuclear decommissioning, waste management, environmental remediation and fuels management (safeguards).

3. Overview of modelling methods in NDA

This section is intended as an introduction to how the various code types are used, and how the results are employed with regard to the end use.

Modelling codes are used for a variety of NDA applications, as indicted in sections 1 and 2. Invariably, codes are used to determine the response of a detector(s) to a specific source of radiation. This is useful for various purposes:

In the design of an instrument, it is possible to use codes as predictive tools, so that the effect of variations in specific design parameters (detector dimensions, geometry, waste container geometry, etc) on the response to specified sources of radiation, can be investigated. This allows the optimum system design parameters to be determined for a specific application, so that the modelling code is used as a design tool. However, in such applications, the validity of the modelling code predictions is not crucial with regard to the validity of the output results of the system, provided that the system is

calibrated in the traditional manner, using physical radionuclide (β/γ) sources or nuclear material (usually plutonium / uranium).

The other main application area for modelling codes, is in the direct calibration of NDA instruments. In these applications, codes are used as a direct replacement for physical radionuclide sources and / or nuclear material. This represents a substantial diversion from traditional methods relying on physical reference standards. However, the decreasing availability of such standards, combined with the increasing accessibility of powerful computing technology, increases the arguments in favour of this method. The advantages are obvious, in that physical reference standards are no longer required. However, the disadvantages are obvious, since the confidence that is obtained by calibration with real physical standards that are known to be highly representative of the actual material to be measured by the system, is absent.

There are various NDA applications where modelling codes are being used increasingly in support of direct system calibrations. It is incumbent upon the organisations that perform such system calibrations, to ensure a high degree of confidence in the validity of the predictions from the modelling codes. This confidence comes from a number of technical and non-technical factors, including the following: appropriate definition of the modelling objectives, operator training, Quality Assurance procedures, model validation / benchmarking, appropriate physics techniques and use of nuclear data, and treatment of modelling uncertainties.

In summary, the application areas commonly covered, include the following.

- Instrument design.
- Instrument performance modelling (sensitivity studies etc.).
- Calibration (absolute, relative, and extending calibration ranges by way of extrapolation or interpolation for example to extend the calibration based on ^{252}Cf measurements to Pu items with different shape).
- Calculation of correction factors (for example self-absorption factors in gamma spectrometry, self-shielding factors in active neutron counting, neutron self-multiplication in passive neutron counting, relative responses for different waste matrices) for which measurement with representative physical standards is impractical.
- Assessment of shielding / background / interferences such as cosmic-rays.
- Specialist expert review assessments / Interpretation of unusual assay results.
- Characterisation of items (e.g. Burnup codes for inventory / SNF).
- Uncertainty assessments (by calculating range of response for different conditions, such as container wall thickness, waste matrix, source distribution).
- Calculation of spectrum shapes for specific measurement scenarios.
- Assessment of effects of design changes to assay system performance, for example source spectrum tailoring, and effects of changing the detector geometry.
- Calculation of effects of source spectrum tailoring, on instrument performance.
- Shielding calculations for radiation safety studies (calculating the dose rate as a function of source – detector geometry and different complex shielding configurations).

Below, we present a number of examples which describe the way that modelling codes have been used to tackle a range of different types of problems.

In addition to these common applications of system calibration and sensitivity studies, NDA system designs sometimes employ modelling codes embedded within thee core software / analysis engines. For example, some gamma scanning systems such as the Tomographic Gamma Scanner [3] employ ray tracing codes for assessment of waste container matrix attenuation properties.

The most widely used Monte-Carlo code in the field of nuclear material measurement is MCNP [4].

Other widely used Monte Carlo codes include MCBEND [8] and TRIPOLI [9] and the GEANT system used at CERN [10].

3.1. Example 1: Calibration of neutron counters using Monte Carlo

One of the main applications of numerical simulation of NDA techniques is the calibration of neutron counters.

The main complication in the calibration procedure of NDA techniques derives from the extremely high sensitivity of these measurements to a lot of parameters: geometry (shape and dimension), chemical/ physical form, container, impurities. An accurate calibration procedure requires a set of standards being as similar as possible to the samples to be measured. This means that a large variety of refer-

ence materials have to be produced to represent all the possible items of the nuclear fuel cycle subject to accountancy verification. The geometry of the sample, for instance, has a big importance on the response of neutron counters. Generally different calibration curves have to be established for each type of container. Presence of other materials in the sample matrix and/or in the container walls affects as well NDA measurements. Heavy materials shield gamma rays, whether light materials moderate neutrons changing dramatically their behaviour. Even the presence of determined elements (like boron, beryllium, and cadmium) as impurities at trace level can perturb the result. Uranium enrichment and plutonium isotopic composition introduce a further parameter influencing the measurement and contributing to the proliferation of standard requirements.

Due to the high number of (sometime costly) special fissile reference materials required by NDA techniques, it becomes fundamental to investigate and develop methodologies giving the possibility to reduce these requirements. Here is where computational methods, and in particular Monte Carlo simulations, can play an important role. Having a suitable model for instrument simulation, it is no longer strictly necessary to have a reference material identical to the sample for instrument calibration. A single well-characterised standard can be used as a representative of a wide class of "similar" items and to establish a "basic" calibration. Then it is possible to compute with the Monte Carlo the deviation from the ideal behaviour (represented by the basic calibration curve) due to the presence of relatively small differences between the real sample and the standard: geometry, presence of other elements, different chemical/physical properties, effect of isotopic composition, etc. Another possibility is to use calculations to extrapolate an experimental calibration curve beyond the boundaries fixed by the available standards.

We call this first lower level "**soft**" application of calculation to the calibration process. The calibration procedure is still strongly relying on experimental data. Calculations intervene only at a "**relative**" level producing just corrections to the experimental calibration. Since the correction factors are generally second order terms of the basic response function, the accuracy requirements for the calculations are not so demanding. For instance when the effect of the simulated deviation from the experiment is lower than 10% of the global instrument response, an accuracy of a few percents in the relative correction factor is certainly enough.

Nevertheless there could be situations where calibration standards identical, or even similar, to the item are not available. In this case the experimental calibration is impossible and we need to establish a calibration procedure entirely based on computational modelling. We call this extreme case "**hard**" application of calculation. Of course, no matter how much we can trust our confidence in our modelling capabilities, a totally blind application of a computational calibration would be extremely dangerous. Before any use of Monte Carlo for "**absolute**" calibration, the model has to be extensively validated. A wide series of experimental measures have to be simulated in order to confirm the quality and to assess the accuracy of the computational model.

An intermediate case between the "soft" and "hard" extremes happens when a single standard is available allowing the measure of a single experimental point. In this case the full calibration curve has to be produced by calculations and the experimental point provides the validation. In alternative the computed curve could be adjusted or re-scaled to fit the experimental point.

Of course the accuracy required for an absolute calibration is much higher than in case of relative applications. The performances of the computational tool should be as close as possible to the results expected from an experimental procedure, that means of the order of 1% or better. This is today at the limit of Monte Carlo capability, but we expect to improve this situation in a near future, mainly through a reduction of uncertainties on nuclear data. An extensive use of "hard" computational calibration could be soon a reality and a standard widely accepted procedure.

Modelling is used to reduce reliance upon representative calibration standards, reduce calibration resource needs (manpower) and reduce overall costs. Recent developments and successful benchmarking have shown that such "**hard**" calibrations can be used, under some conditions, with confidence, thus removing the need for absolute reference standards (such as fissile material). A common practice in modelling neutron counting systems is to use calibrated neutron sources (that is, with known neutron emission and purity) instead of Pu standards. For example, ^{252}Cf spontaneous fission sources have a spectrum very close to that of Pu and can be used as "transfer" reference standards. They can be used to conveniently represent dispersed Pu (the small physical mass gives rise to negligible self-multiplication and self-shielding effects). Modelling is therefore often performed to simulate experiments with a ^{252}Cf source, for benchmarking and sensitivity studies.

Monte Carlo modelling is most widely used for modelling of neutron assay systems – the established code MCNP [4] being perhaps the most widely used.

3.2. Example 2: Typical approach for in-situ gamma spectroscopy modelling

Modelling codes are often used to perform efficiency calibrations in support of quantitative gamma ray spectroscopy measurements, for example in decommissioning and waste management. Examples include measurements on plant items with geometries for which it is prohibitively difficult to construct a calibration geometry with the appropriate distribution of sources, such as heterogeneously filled waste drums, and bulk waste items from decommissioning operations.

It is possible, using commonly available codes, to use computer modelling techniques to calculate the efficiencies for such geometries, thereby permitting quantitative analysis. Modelling tools allow various geometries to be modelled including different shapes of item, container fill – matrix, and source distribution, together with options for the detector details and shielding / collimation.

By modelling the range of such parameters, it is possible to study in a systematic manner, the effects of varying key geometry parameters, on the measurement results, in order to estimate the measurement uncertainty. Such studies are not generally practical by measurement, due to the difficulties associated with arranging appropriate sample / source geometries.

Various techniques are used to perform such calculations, including Monte – Carlo modelling (codes such as MCNP [4] and MCBEND [8] and TRIPOLI [9]) for the detector response function, and “line of sight” attenuation models (codes such as ISOCS [5, 6 and 7] and MERCURAD [11 and 12]) to determine the sample attenuation and sometimes the detector response function (the “MERCURE v6” software is distributed by Canberra through the “MERCURAD” human graphical interface). As for neutron applications, it is crucial to ensure that particular measurement applications are performed within the defined dynamic range of for which the modelling has been benchmarked and for which code validations, exist. References [5 and 21] provide examples of these activities.

With recent advances in modelling methodologies, it is becoming common to model full pulse height spectra (to predict performance under realistic field conditions), as well as calculating full energy peak efficiencies and relative efficiencies.

3.3. Example 3: Typical approach for reactor physics codes

Reactor physics codes in support of NDA measurements are mostly used to compute the composition of irradiated materials. In fact, it is often very difficult (or mostly impossible) to measure the mass of nuclear material in irradiated fuel. This is due to the fact that differently from fresh nuclear material where the spontaneous fission neutrons are generated basically from plutonium and can be used for quantitative assay of plutonium mass, in spent fuel the dominating neutron signal comes from (even very small amounts of) curium and overwhelms the plutonium signal. Therefore, being the direct measurement of SNM impossible, most of NDA techniques aim to the confirmation of the fuel burnup through the measurement of Cm-generated neutrons or of fission product photons and the amount of SNM is therefore inferred through the calculation of spent fuel composition using isotopic generation/depletion codes.

The historically most used among this family of codes is ORIGEN [14]. It solves the huge system of differential equations describing the time evolution of any number of isotopes accounting for all types of nuclear decay chains and neutron induced reactions. The use of this code is relatively straightforward and accessible for users who are not specialist in nuclear physics. In fact most of the required input is "objective": that means it requires mostly physical data as initial composition and irradiation history (time and flux or specific power). The major limitation of ORIGEN derives from the availability of nuclear data. In fact, in order to solve the evolution equation accounting for neutron induced nuclear reaction, the code needs to know the 1-group neutron cross sections for all isotopes. To obtain an accurate 1-group cross section set, it is necessary to collapse energy-dependant or multi-group cross sections to 1-group by weighing on the energy spectrum of the neutron flux. This step is very delicate and requires the use of sophisticated models and codes and a deep knowledge in nuclear physics. For this reason the normal approach is to have libraries developed by specialists who can produce dedicated cross sections sets for any type of reactor and fuel. Normally ORIGEN (or similar codes) is distributed together with a wide set of cross section libraries covering the most typical cases and matching the most frequent needs. Nevertheless no library set can be fully comprehensive and it may happen

that a specific case is not included. In this situation it is responsibility of the user to select the most suitable library among the available ones, to be aware of the possibility of biases, to assess the related uncertainties and possibly to validate or benchmark the code+library versus experiments for the specific type of reactor and fuel.

To overcome the limitation of the availability of a suitable cross section library, some more recent codes implement the possibility to generate directly the problem-dependant cross sections. An example of this family is SCALE [15]. SCALE is not a simple code, but a modular system. This means that it is a collection of several codes, each one performing different tasks with a standardised input/output system that allows one to enter automatically the output results of a module as input data of the following one. So the single codes (called functional modules) can be executed either in the traditional stand-alone way or linked together in a cascade of modules each one using as input the results of the previous codes. Special super-modules (called control modules) allow one to build automatically pre-determined standard sequences of functional modules. The system is provided with other ancillary modules performing utility tasks as data management, and with an extended set of libraries containing nuclear properties, cross sections, material properties. One of the SCALE sequences, SAS2H, is explicitly designed to perform burnup calculations. It uses the description of the fuel assembly in order to compute the neutron spectrum in the cell, to collapse the cross sections and generate the specific set of nuclear data (see Figure 1).

This approach enlarges the applicability of the code to potentially any type of burnup calculation. The disadvantage is that the use is more complex: the user becomes responsible for the modelling of the reactor and fuel and for the choice of the appropriate methodology. This latter in particular requires the selection of options about algorithms for neutron flux calculation in the fuel cell, self-shielding treatment, homogenisation and energy collapse. This choice is no longer based on purely objective physical data, but relies on the knowledge and competence of the user introducing a sort of subjectivity. SCALE and similar systems can be much more accurate than simple ORIGEN-type codes, but they are at the same time more delicate and much more depending on the user capability and training.

3.4. Example 4: Combinations of different codes / techniques

A classical example of combination and integration of different measurement techniques and analysis

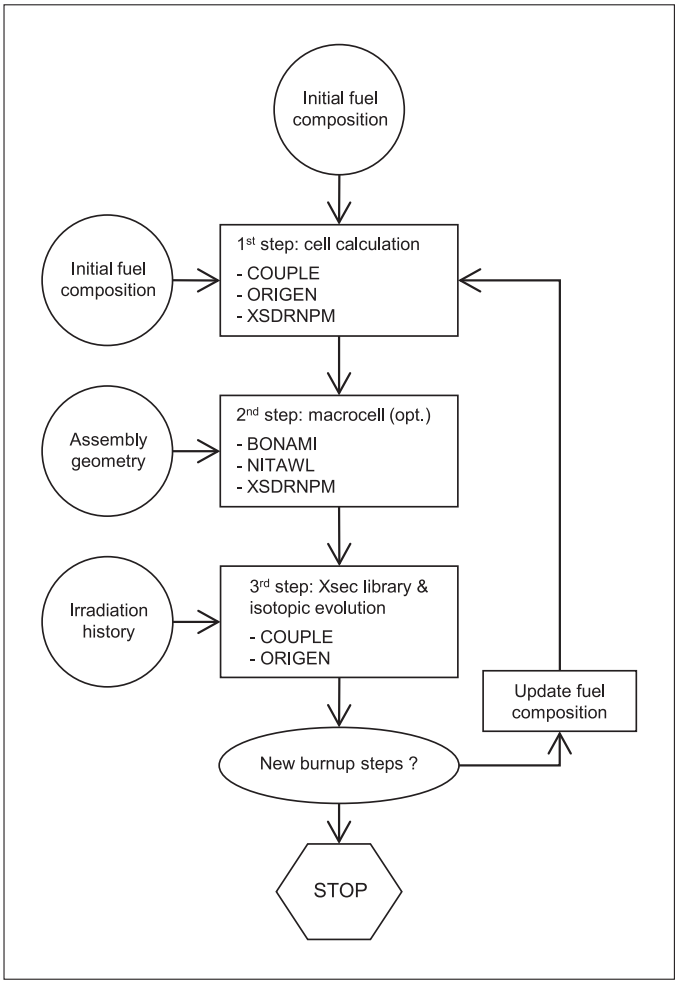


Figure 1: Flow-diagram of the SAS2H sequence in SCALE for burnup calculations.

codes is the FORK detector used for spent fuel verification.

The Fork Detector Irradiated Fuel Measuring System shown in Figures 2 and 3 incorporates in its detector head gamma ray insensitive neutron detectors (four gas filled fission chamber proportional counters) and gamma ray detectors suitable for measuring extremely high gamma ray intensities (two gas filled ionization chambers). The neutron and gamma ray signatures measured by the detectors are used to verify the highly radioactive spent fuel assemblies stored underwater in spent fuel ponds. The FDET is positioned about 1 m above the tops of neighboring assemblies. The irradiated fuel assembly being measured is lifted so that the tines of the detector straddle the fuel portion of the assembly in order to collect the neutron and gross gamma data.

In the FORK detector the ratio of the neutron to gamma ray data, when combined with other, complementary information, is used to characterize a particular type of fuel assembly, giving information related to its neutron exposure in the reactor, its

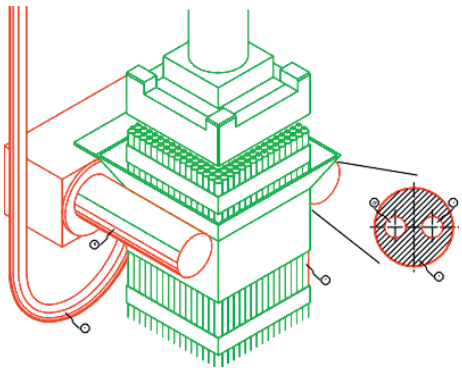


Figure 2: Drawing of the FORK detector during safeguards inspection measurements. In red: the FORK detector, in green: the fuel assembly to be measured.

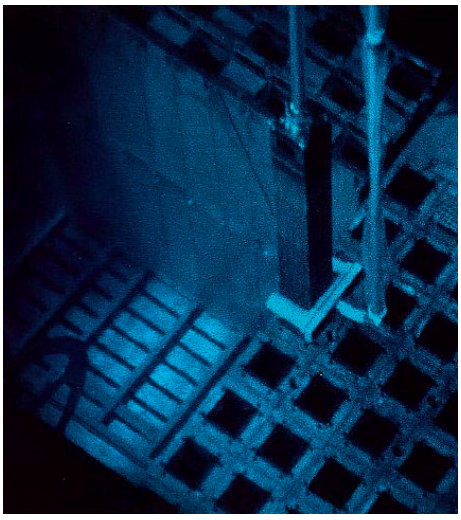


Figure 3: Fork detector during safeguards inspection measurement [16].

initial fissile fuel content and its irradiation history (e.g. the number of cycles for which the assembly was in the reactor). The gamma radiation is dominated by the fission products, mostly ^{137}Cs in aged spent fuel. The neutron signal is determined the Cm and Pu isotopes, but in large majority is due to ^{244}Cm. The confirmation of operator's declaration of the initial composition, fuel burnup and cooling time is done by comparing the neutron and gamma radiation measured by the detector with the expected composition of the spent fuel computed with inventory codes, such as those described in example 3. In parallel the detector calibration (that is conversion of ^{244}Cm mass in neutron count rate) can be done with Monte Carlo codes as described in example 1.

The SMOPY system [17] is another system used for fuel verification measurements. This system uses a combination of neutron and gamma detection to measure the burnup. The methodology combines measurement of the total neutron emission rate, with the fission product yields and modelling using the CESAR code [18], for burnup measurement applications such burnup credit assessment.

Combinations of codes are often used for various combined reactor physics applications, for example the CRISTAL code system [19] which uses a combination of the APOLLO, TRIPOLI and MORET codes.

For decommissioning applications, combinations of measurement techniques / modelling codes are sometimes combined to develop an integrated measurement solution. An example is the combined use of dose-rate simulation with modelling to determine the response function of a detector for a particular geometry. Gamma imaging can support such studies, in order to determine, for example, the locations within a plant glovebox containing the highest concentrations of holdup. Dose-rate modelling can determine the operator doserate at particular locations, whilst calculations of the detection response function (with a code such as ISOCS) can allow the activity of measured nuclides, to be quantified. Such modelling allows can allow, for example, glovebox dismantling operations top be optimized, reducing operator doserates whilst providing activity assessments for plant items. Examples of such approaches are given in [12 and 13].

4. Best Practice Methodologies

4.1. Problem Definition

Before a modelling campaign can proceed, it is vital that a clear understanding is formulated, of the objectives of the work. The nature of the objectives can heavily influence the modelling techniques deployed.

It is recommended that the objectives are clearly documented, to enable the modelling campaign to be conducted properly. Common objectives include the following:

1. Determination of optimum geometry for a particular NDA system design, by making incremental changes in the model to key system parameters (it would probably be extremely impractical to make these adjustments experimentally).
2. Investigation of the variability in response of a system, to well defined variations in sample – specific parameters (for example fissile material mass / nuclide activity, waste container dimensions, waste matrix composition, etc.).

3. Direct calibration of an NDA instrument, to determine the relationship between the source activity (or mass) and the measurement response.
4. To determine a set of sample – specific parameters that are related in some way, to the results of an NDA measurement.

These objectives may each require different techniques to be applied, in the use of the appropriate modelling codes.

When used for design of NDA instruments, the results of the modelling are only applied in allowing the system design to be optimised, in a systematic manner that would not have been otherwise possible. It is only the instrument design itself, that has been influenced by the modelling. For these design applications, there are less stringent requirements on the modelling practitioner, than would be the case for direct calibration applications, for example. The designer must have a certain level of confidence in the results of the modelling, in order to avoid expensive mistakes in the system design. However, use of the modelling in this way does not have a direct impact on the output results of the NDA system. For such design applications, designers often use elaborate features of the applicable codes (e.g. variance reduction techniques) to optimise the design process.

Codes can be used in a predictive manner to predict the variability in response of a system to identified changes in specific sample parameters. In such case, the codes are used to illustrate the variability in response or output quantity (e.g. mass or activity), but only for illustrative purposes. The results of this modelling may influence the schedule for a measurement campaign later, but they do not directly affect the output result of the system itself. Modelling may be deployed in such a manner, in order to design a measurement campaign, for purposes of recalibrating an NDA system, for example. However, the subsequent calibration campaign would then invariably be subject to its own procedures. In these applications, it is obviously important that experience has previously been built up in the use of the code for the particular application. The consequences of not adopting best practice, could be delays to measurement campaigns, perhaps requiring additional radionuclide sources to be procured, with the obvious associated “knock-on” costs.

It is when modelling is used for direct calibration of NDA systems, that the modelling results have the highest importance. In these cases, the modelling has a direct effect on the output of the NDA system. The consequences of not adopting best practice methodologies, are obviously potentially the most serious, in these cases. One is relying on the modelling to determine the relationship between the source-specific parameter (usually activity or fissile mass) and the measurand. Particular emphasis is placed on benchmarking, when modelling is used in this way. It is particularly important that the benchmarking has been demonstrated to be applicable across the full dynamic range, wherever possible. In practice this usually means that a particular modelling technique should be benchmarked to show good agreement between experiment and model, over a measurand range equivalent to that for which a new calibration is being developed. It is also appropriate to consider new benchmark campaigns, for example when a code methodology (such as coincidence counting) is to be applied for a new type of fuel assembly.

Some modelling codes are used indirectly, to relate the output result of an NDA system, to some other quantity. The most common example of this is reactor physics “burn-up” codes. In these codes, it is common to relate, for example, the ^{137}Cs activity (which is often readily measured by an NDA system), to the activities of various other un-measurable β/γ nuclides and actinides. In such cases, the (otherwise unrelated) result of an NDA system is combined with the results of the modelling code, to yield nuclide activities, which may later be used for waste sentencing purposes. A similar level of stringency is therefore required, as for calibration applications, and benchmarking should be considered as equally important.

In documenting the problem definition, consideration should be given to the existence of relevant benchmarks, and whether any further preparatory benchmark work is required before a specific modelling campaign can proceed.

The following aspects should be considered, as a minimum, when documenting the requirements of a specific modelling campaign:

- What is the end-use project / who is the customer?
- Is the modelling related to an existing NDA system (in which case, is there an existing model), or a new system?
- What is the range of sample – specific properties to be considered?
- What quantity is to be calculated?
- How are the results to be used?

- What accuracy is required for the calculated results?
- What precision is required for the calculated results?
- How are the modelled quantities to be converted into NDA system output quantities (e.g. combination of MCNP calculated quantities to produce the neutron counter "Reals" coincidence count rate)?
- How are the results to be reported?
- What benchmarks exist?
- Are new benchmarks required?

These considerations can determine the modelling techniques to be used. For example, it is possible that documented benchmarks relevant for the specific application, show that it is not possible to achieve the required accuracy, and further benchmarking must be sought. The required statistical precision has a large impact on the length of time to be assigned to the models.

If the results are to be used to calibrate a safety – critical NDA system, there may be specific plant requirements that dictate a higher level of stringency with regard to calibration validation.

4.2. Benchmarking / Validation

One of the most important factors regarding the correct use of modelling in support of NDA system calibration / performance testing, is to ensure that the system model is appropriately benchmarked against experiment. In practice, this means that a benchmark measurement is performed, under typical conditions for the NDA system, and a model is performed under identical conditions. Comparing the measured and calculated system response, allows an assessment of the level of agreement, to be performed. The problem definition phase of a modelling campaign should define the level of benchmark agreement, that is required for a specific application. Modelling results can be renormalized, to take into account any such bias.

Benchmark experiments are used to compare the modelled / measured response for a wide range of geometries, designed to simulate various applications. It is crucial to ensure that particular measurement applications are performed within this defined dynamic range, for which established benchmarks and code validations, exist. Reference [5] gives a set of example benchmarks for the widely used ISOCS system, while references [20] and [21] provide example benchmarks for the commonly used MCNP code.

It is vital that the validity of the model is confirmed throughout the dynamic range of the parameter space to which the model will be implemented. For example, if modelling is being used to determine the effect of a drum matrix on a PNCC system response, then one should devise a benchmark experiment using a matrix which leads to a system response representative of the range of real matrices. This means that a benchmark is required which represents the typical range of measurement conditions. In practice, if the modelling and measurement results show a discrepancy of say 10 %, this can be interpreted as a fixed bias, and it is therefore appropriate to apply this factor as a normalisation constant to all results predicted by the model, if the results are to be used to calibrate an NDA system. In the above example, if the real range of matrices produces a modest variability in response, to say ± 20 %, then a single benchmark with a typical matrix within this range, would suffice. However, it would not be sufficient to assume that the same benchmark test is still valid, if a model is to be applied to the same system with a grossly different geometry, for which the response has changed substantially (e.g. changing to cadmium liner mode in active neutron NDA systems).

If a model has been obtained from a contractor or other external organisation, then an appropriate benchmark should be sought, prior to use of the model. Sometimes, this can take the form of appealing to a publication in the open scientific literature, or a referenced communication with the contractor.

It is recognised that it is not always practical to obtain benchmarks that comprehensively cover the full dynamic range for a parameter space of interest. For example, it may not be possible to obtain a benchmark for an enrichment value for a new fuel element type, because it is impossible to perform a benchmark experiment when a physical sample is not available. In such circumstances, a technical assessment should be performed, to assess the impact of this lack of availability of benchmark experiment data. This may include, for example, inspection of the nuclear data, and an intelligent assessment of whether the extrapolation to a new enrichment value (in the case of the example above), is likely to have any significant impact.

Another example is the use of MCNP to extrapolate to new fuel types, and / or extrapolating to higher masses for which benchmarks do not exist. This

approach may be justified, provided that one has a lot of confidence in the physics methodologies and the validity of the nuclear data used. For example, special physics studies can be performed, to validate such extrapolations.

Published benchmarks exist for widely used codes. For example for MCNP, a large number of benchmarks exist for neutron and photon applications [see references 20 and 21 respectively]. For specific NDA application areas such as nuclear fuel verification by PNCC assay, special benchmark projects are typically organised [see references 22, 23 and 24]. Similarly, benchmarks exist for the gamma-ray attenuation modelling code ISOCS and others [see references 25 and 26]. ISOCS is widely deployed for calculating the efficiency of detectors for difficult geometries for which it is impractical to construct representative physical calibration standards.

4.2.1. Case- Study 1: Calibration of neutron counters at JRC

JRC has performed calibrations for DG-TREN (Euratom Inspections) and for the IAEA to provide calibrations of various neutron coincidence counting systems for different applications where suitable reference materials for experimental calibration were not available. The description of the different problems, of the proposed solutions and of the obtained performances and results are documented in references [27, 28, 29, 30, 31, 32 and 33] and cover several applications:

- measurement of HEU fuels with extremely high ^{235}U linear masses
- extension of calibration curves of collars for LWR fresh fuel assemblies with higher ^{235}U enrichment
- calculations of correction factors for burnable poison in various conditions
- calibration curves for VVER fuel assemblies
- use of AWCC for special HEU rods
- passive collars for magazines of MOX fuel rods
- passive neutron scanner for “chaussettes” with several boxes of PuO_2 powders.

We want to summarise here the basic concepts that were applied and the operational procedure followed in all these cases. This procedure could be used as an indication of good practice for this kind of application. The basic procedure applied at JRC is based on the following steps:

- measurement in the PERLA laboratory of a large set of reference standards with the same detector (and eventually the same source for active systems) to be used
- comparison between Monte Carlo calculations and the experimental results in order to validate the computational model of the detector
- generation with Monte Carlo calculations of the response function of the detector with the special type of samples
- on-site verification of real samples.

The development of an accurate model for the neutron detector is the most important and delicate task of the entire procedure. The first two steps aim to the validation of the computational model of the detector. Once a fully validated model of a counter has been properly benchmarked, this opens theoretically the path to the calibration for any kind of sample. Indeed the first two steps validate at the same time the model of the detector and the models of the reference samples measured in the laboratory campaign.

It remains questionable how much is reliable the development of the Monte Carlo model of the special samples for which the calibration has to be computed in the third step. This is much harder to be proven and it is possibly the weakest point of the suggested procedure, since there is no a-priori way to guarantee the quality of a new model. Of course the situation will be much better when the reference materials used in the first steps are very similar to the special samples: in particular when they have the same geometry, since the geometry is the most delicate parameter of a Monte Carlo model, where it is higher the probability of making errors. For instance, in the case of the extension of the calibration curve of fresh fuel at higher enrichment, the geometrical model of the PWR and BWR fuel assemblies had been validated in the first phase with respect to real measurements, so the extrapolation to higher enrichment (involving only the modification of the material composition) was straightforward and error-proof.

Recommendations from user experience:

Trying to generalise the outcome of the experience coming from the analysis of a large set of comparisons between calculations versus experiments with neutron coincidence counters, we can draw some general remarks:

- the accurate description of the geometry (dimensions, compositions, density) of the detector is of paramount importance

- do not rely on construction drawings and information provided by the manufacturer, but get the above mentioned parameters by direct measurement
- agreement is generally better in cadmium lined detectors (fast or epithermal neutron spectrum) than in fully thermalised assemblies, this suggests some refining could be needed in the cross sections of polyethylene, probably in the S(α,β) treatment [4] and in the influence of temperature
- for passive systems one of the main sources of error comes from nuclear data – 1% in the spontaneous fission half-life gives directly an uncertainty of 1% on efficiency and therefore on Totals and 2% on Reals
- we know the multiplicity distributions only with high uncertainties
- in active systems we have also to add the limited knowledge on the interrogation (Am,Li) source spectrum, especially in the low energy tail.

Practically we can conclude that the accurate knowledge of nuclear data is currently the bottleneck for the performance of Monte Carlo modelling of neutron counters.

4.2.2. Case- Study 2: Benchmark exercises performed for neutron safeguards assay

In recent years, three benchmark exercises have been organised, to establish the performance of Monte Carlo modelling techniques as applied to the safeguards assay of fissile material. These followed the gradual development and improvement in availability of modelling hardware, and sophistication of interpretational models. These projects include the following:

- Reals Prediction Exercise [22]

  This project compared a wide range of Monte Carlo modelling codes and interpretational models, applied to calculate the Reals response for a PWR fuel assembly in an AWCC collar. The project highlighted the level of agreement that could be achieved using the modelling tools available at the time, and demonstrated the importance of nuclear data in producing accurate results. At the time of this project, most of the interpretational models were based on point model approximations.

- Simple Case Benchmark [23]

  This project was based on a simple neutron slab counting geometry and compared the use of different Monte Carlo codes to calculate the efficiency for a calibrated, traceable 252Cf radionuclide reference source. The results were compared with the measured efficiency. A 252Cf source was used because such a source is often used to measure and calculate the efficiency for benchmark systems, to allow Monte Carlo modelling to calculate calibration parameters in a "relative" sense. The analysis focussed on the effects of different codes, physics treatments and nuclear data. The importance of the nuclear data was shown, in the context of the fundamental limitation that these impose on the accuracy with which modelling tools can calculate absolute responses. Areas for further development were recommended, for example in the evaluation of a consensus source spectrum term.

- Multiplicity Benchmark [24]

  With the increasing availability of powerful computing platforms, it is now possible to simulate directly, through Monte Carlo modelling, the response of neutron coincidence and multiplicity analysis electronics, rather than relying on the intermediate stage of the interpretational point model which necessitates inherent approximations. This benchmark project is directed at the establishment of a standard modelling code and methodology, which is capable of direct simulation of all of the aspects of neutron coincidence / multiplicity analysis systems (efficiency, deadtime, multiplicity distributions and moments, etc.).

4.2.3. Case- study 3: Validations for gamma spectrometry waste measurements [5 and 13]

For in-situ gamma spectroscopy modelling codes a large number of published benchmarks exist (see, for example, references [5 and 13]). However, in view of the versatility of the modelling codes, it is important to be aware of the magnitude of the uncertainties, and the effects of the approximations and assumptions that are made when modelling both the geometry of the physical item to be measured and the spatial distribution of the activity within it. For this reason, it is important that the validation carefully bounds the specific assay problem. This is particularly important when seeking regulatory acceptance of proposed methodologies.

Typically, in the fields of decommissioning and waste management, validation exercises for gamma and neutron assay applications are performed on a project-specific basis, recognising the unique na-

ture of many projects and waste streams. Validation often includes the construction of inactive simulated waste containers with re-entrant tubes inserted, allowing placement of radioisotope standards at well defined positions covering the full range from best to worst case measurement scenarios. Comparison of measurement and calculation then allows a validation to be made for the modelling process. In this context, the terms “validation” and “benchmark” may be used interchangeably. Other validation methods are sometimes achieved through the use of sampling and laboratory analysis. For example, when measuring bags of (homogeneous) soil by in-situ gamma spectroscopy, it is possible to take small samples from various positions throughout the bag. The specific activity of these samples is then measured by laboratory techniques, and compared with the overall specific activity for the bag as measured by the in-situ technique.

4.3. Training / Competency

When modelling a physical problem, the quality of the result is a combination of three main components:

- the use of a **code** implementing accurate mathematical models adequate to describe the physical reality coupled with efficient algorithms to solve the mathematical equations
- the use of a set of best available **physical data** (such as nuclear cross sections) describing the material properties at the best of the current knowledge
- the representation of a system using an appropriate geometry model and physical treatments
- an experienced and competent **user**.

The human factor is probably the most difficult component to be assessed. In fact the typical accuracy of a method can be evaluated through an appropriate benchmarking campaign and the influence of uncertainties on nuclear data can be derived by a sensitivity analysis. There is no way to evaluate a priori the effect on the result of a poor or experienced use of a code.

The ideal user should:

- be capable to understand all the implications and consequences of the choice of any parameter that the code leave free to be set by the user
- utilise in an optimal way all the possible options and approximations offered by the technique
- describe the physical model with the highest accuracy reasonably achievable, using simplifications only when clearly demonstrated to be not influent
- assure that assumptions and simplifications affecting significantly the result are made only in a conservative way, when this concept is applicable (for instance in criticality evaluation and dose estimation).

Any quality assurance systems require that any operator performing a task is competent and trained to do it. This applies also to the use of codes and physical models. Any individual using a code should have gone through a complete training process including:

- having an appropriate educational background
- participation to dedicated/specialised training courses
- on the job learning with tutoring from other experienced user(s).

Training itself does not guarantee the correct application of the acquired generic knowledge to a specific problem. The human factor can be improved only through a complete validation process involving the entire (code + user) system. In section 4.2 we have described how a code can be assessed and validated through a large number of comparisons between calculations and experimental data. Indeed each user should run himself at least a limited number of benchmark cases in problems that are as close as possible to the problem to be solved in order to prove and validate its own capability to model adequately the problem.

4.4. Quality Assurance

This section is not intended as a prescriptive step-by-step procedure. In practice, modelling codes are too complex to simplify along these lines. Instead, the procedure gives general guidelines which, if followed by specialist NDA staff, will ensure a high degree of confidence in the validity of the results produced. In any case, NDA specialist staff will be fully trained (see section 4.3) and competent in the details of the modelling process, through a combination of experience, and a working familiarity with the operations manuals prior to engaging in any work.

It is important that practitioners of modelling codes take care to ensure that careful records are kept of their modelling work. This ensures traceability, al-

lowing modelling programs to be recreated by others, and ensuring repeatability.

It is recommended that dedicated logbooks are used to record the working details associated with model development, and for recording input and output data. These logbooks should also be used to record all relevant data and information associated with a modelling program, as described in this document.

For large modelling campaigns, a model specification document may be produced, providing a template for running the models, and recording results. This approach is useful if the modelling is to be performed by a team of physicists. The model specification document should contain information such as the geometry models and source descriptions required, the output data required, the format of the results, and the precision requirements (relevant for stochastic modelling codes such as MCNP). This approach can greatly assist the peer review and auditing processes, for applications where a large amount of data is created.

Typical contents of a modelling specification document are:

- Reference to benchmark applications, demonstrating the validity of the code, for the parameter range of interest.
- Reference to benchmarked model which is available, from which a new model for the present application, can be derived, with minimum extrapolation / interpolation.
- MCNP models produced for similar applications in previous work.
- Relevant technical reports produced in previous work.
- Details of parameter variations required.
- Details of output tallies required.
- Details of recommended analysis procedure / interpretational model to convert from model results to system response.

Typical outputs from a modelling program are:

- Checked and Approved Models (MCNP Input Files).
- Model Checking Records.
- Modelling Results (MCNP Output Files).
- Data analysis spreadsheets etc.
- Analysis results including description of the interpretational model used to convert the raw output tally from the mode, into a system response quantity (e.g. count rate).
- Technical report.

The data to be included in the logbook should include the following information:

- Each page should be numbered, and labelled with a project reference.
- Author.
- Date.
- Reference number to the particular project that the model relates to.
- Reference to a previous model (from which a new model is developed), if applicable.
- Reference to relevant section of modelling specification.
- Description and sketches describing the model geometry development, allowing a reviewer to follow the model development.
- Change history (differences between models as they are developed).
- Model description, including details for the following:
  - Source term (position, energy spectrum, directionality, etc.).
  - Materials used for the various parts (cells) of the geometry.
- Full references should be given to supporting data used to develop geometry models and physics modeling techniques, including engineering drawings, measurements, technical papers, etc.
- Records of assumptions / approximations made in setting up the models.
- Details and justifications, for all departures from normal practice (for example, the use of special variance reduction techniques in MCNP).
- Record of the version of the code being used.
- Details of, and reference to, all nuclear data used (e.g. fixed library supplied with the code).
- Comments throughout.
- Records of model filenames (input and output files), and directory path structure.
- Records of filenames for analysis programs and spreadsheets etc.
- Details of computer run times as appropriate.

- Details of output results / tallies, and uncertainties.
- Derivation and statement of "fitness for purpose" of modelling technique depending on the end-use and consequences (for example with regard to the effect on the output of a measurement system).
- Record of peer review of models.
- Record of any manual "check" calculations / spreadsheets which might be performed in order to add confidence in the validity of the modelling code results (for example it is common practice, when setting up new modelling approaches, to check the validity of the results incrementally, to build up confidence in each new stage of the approach).

Model checking:

During the development of a geometry model for an NDA system, full use should be made of any in-built or subsidiary geometry debugging facilities. These may allow detailed views to be displayed, with graphical indications of areas with erroneously defined geometry. Examples include the MCNP-VISED program, available with the most recent distributions of MCNP.

Models should be checked and validated ("peer reviewed") by a physicist, qualified in the operation of the particular modelling code and procedure. Model checking records sheets may be used as appropriate to provide evidence that the checking and validation has been carried out correctly.

Typically, when developing a geometry model for a system which is to be used to perform calibrations, model development should proceed (recording full details of the model development process, in the logbook) until a base model has been developed, for which it can be demonstrated that adequate benchmarking agreement can be obtained, with experiment. At this stage, the model should be "frozen" for future reference, and subject to peer review. Normally, parameters of interest (e.g. waste drum dimensions, source geometry, fuel element enrichment, etc.) are then varied, to perform the modelling campaign (it is not normally required to perform peer review for each of these individual models). When used for calibration applications, system details such as the nuclear data libraries, physics tallies deployed, and detector configuration, should not normally be varied at this stage, having frozen the base model. However, when used for sensitivity studies / design studies, it may of course be necessary to make modifications of this kind, in which case additional peer reviews may be performed, depending on the complexity of each particular application.

Departures from established normal practices:

Departures from normal practices (as prescribed in the code manual) should be fully justified and documented. Operators should be fully conversant with the correct methodologies for using a particular modelling code (for example, through completing an MCNP course). It is outside the scope of this document to prescribe specific methodologies for operation of specific codes. However, operators should comply with the conditions of the code manual, which generally reflect a large amount of accumulated experience from a range of operators (for example, using beta-testing, and input from user's forums). All departures from these normal procedures should be subject to written justification.

4.5. Nuclear Data

4.5.1 Introduction

The design, evaluation and interpretation of NDA measurements invariably require basic physical data such as decay data and interaction coefficients to be available. The experimental and theoretical literature on the determination of such quantities as: half-life; decay scheme; energy; branching ratio; photon interaction coefficients; neutron cross-sections; reaction product yields; charged particle stopping powers etc. is vast, in a constant state of change, and can be confusing. The task of collating and evaluating data to create a self-consistent, or at least a screened, reference set is an activity requiring specialist knowledge, experience and tools. It can often be a painstaking undertaking and might best be described as a scientific art.

For the most part, therefore, the selection of physical data is best made from a reputable and recent evaluated source which will be maintained. It should be referenced and remain accessible so that other workers may also make use of it to repeat the calculations made with it.

A physical measurement is meaningless unless it is accompanied by a statement of the confidence in the results. Similarly the data one uses should have an uncertainty assessment associated with it. For some classes of data this may be hard to provide. If the experimental data base is sparse, contradictory and or highly convoluted with other physical data or if theoretical models have been used to guide the evaluation it is often quite difficult to evaluate the

uncertainties objectively. Some evaluators may provide semi-subjective commentary. Furthermore the uses of the data may not result in a simple sensitivity analysis. For example in calculating the slowing down behaviour of fast neutrons in a material the scattering cross section and chemical binding treatment may be sampled many times in a highly problem dependent way. In such cases it is useful to have several evaluated data sets available, perhaps different revisions or perhaps performed by different groups, to use as reference values, and to repeat to calculations to find out what impact a particular choice has. It is also valuable to vary the input data systematically in other ways to determine the sensitivity for the problem at hand.

Accordingly we may think of evaluated data as being a convenient source of reference data. The particular evaluation one chooses should ideally yield results that are acceptable against benchmarks relevant to the problem at hand but it is a mistake to think of a particular evaluation as necessarily the best data. An evaluation provides at best a snap shot which is hopefully reasonably representative of the current state of knowledge. The proof of which data set is better than another depends on detailed comparison against careful experiments and this can be rather difficult to decide. Evaluations of difference provenance therefore have great value in allowing the user of the information to gauge the impact on the final results of interest to them, of the choice of data.

If a system has been calibrated in such a way that it makes use of a particular set of physical data then it is important that the interpretation of the measurements make use of the exact same data in as much as that matters to the outcome. In other words one should be rigorously consistent.

Similarly one cannot change the data used to interpret data arbitrarily as new evaluation become available since, although this may result in a 'better' decay correction, say, it will also result in a discontinuity with what went before and the important purpose of some measurements is to consistently verify the item is unchanged.

Many computational tools have embedded within them data sets which the user can make use of, and the same is true also of some interpretational codes which have preloaded libraries (e.g. MGA). In these cases the user is freed from the burden of searching and selecting suitable sources of data but retains the responsibility of confirming the data is fit for purpose and does not give rise to inconsistencies in use.

The purpose of this "good practice guide" is to provide guidance to ensure that correct procedures are followed in the selection of nuclear data sets, as part of performing modelling calculations in NDA. The important point here, is that one should follow a defined set of principles, in order to provide confidence in the validity of the nuclear data deployed. In practice this includes issues such as what factors need to be considered when selecting the most appropriate nuclear data library, and how these data libraries should be managed.

It is outside of the scope of this document, to prescribe recommended values for specific nuclear data parameters. The nuclear data must be considered as part of a closed system when used as part of a modelling code, and can only be validated as such. However, it is possible, from the extensive benchmark exercises that have been performed in support of the development of modelling codes in nuclear materials safeguards, to comment on areas where further attention is needed., and on exercises which indeed provided useful information on preferred nuclear data sets, in the sense that the best agreement was achieved with benchmark experiments.

We present in references [34, 35, 36, 37, 38, 39, 40, 41 and 42], examples of recent work in the fields of neutron and gamma NDA techniques.

4.5.2. Nuclear data for Monte Carlo simulation of neutron counters

All Monte Carlo codes for neutron transport simulation are provided with cross section libraries. For instance MCNP, one of the most frequently used codes, is distributed with its own set of libraries and continuously new libraries are produced by different laboratories following the demand and the release of upgraded new evaluated nuclear data files (ENDF, JEFF, JENDL and others). A world-wide activity of validation of these data is permanently ongoing.

It is out of the scope of this guide to discuss and analyse the quality of MCNP libraries. Generally speaking, neutron counting requirements are not different from any other application of Monte Carlo codes and no specific improvements are needed, with maybe just the following exception.

All the modelling codes need an adequate description of the medium properties and in the case of codes used in modelling NDA techniques the nuclear data are the most relevant. Often codes are released with their set of nuclear data. Any validation procedure guarantees the correct performance of the code and associated nuclear data, so it has to be considered a unique and compact system. Changing nuclear data will invalidate the passed validation and require a new benchmark of the code with the modified data.

We will provide here a synoptic of nuclear data used in neutron counting. The nuclear data needed depend on the kind of application. For instance they are used by some of the interpretation models applied to process the rough measured data. In this section we will consider the so-called "point model" that is generally implemented in the systems based on the multiplicity counting technique.

4.5.2.1. Models for the interpretation of measured data

The point model is at the basis of the multiplicity counting technique [43 and 44]. It states that it is possible to determine the spontaneous fission rate in a plutonium sample by measuring three experimental quantities (the Singles, Doubles and Triples counting rates) and solving the system of the three equations governing the diffusion and detection of neutrons:

$$S \cong F\varepsilon M\upsilon_{s1}\left(1+\alpha\right) \quad \text{Eq 1}$$

$$D \cong F\varepsilon^2 f_d M^2\left[\upsilon_{s2}+\left(M-1\right)\frac{\upsilon_{s1}\upsilon_{i2}}{\upsilon_{i1}-1}\left(1+\alpha\right)\right] \quad \text{Eq 2}$$

$$T \cong F\varepsilon^3 f_t M^3\left[\upsilon_{s3}+\left(M-1\right)\frac{2\upsilon_{s2}\upsilon_{i2}+\upsilon_{s1}\upsilon_{i3}(1+\alpha)}{\upsilon_{i1}-1}+2\left(\frac{M-1}{\upsilon_{i1}-1}\right)^2\upsilon_{s1}(1+\alpha)\upsilon_{i2}^2\right] \quad \text{Eq 3}$$

where:

F = spontaneous fission rate in sample,
ε = neutron detection efficiency,
M = Total neutron multiplication
(in practice the model requires that the leakage multiplication ML = MT),
α = (α,n) to spontaneous fission neutron ratio,
f_d, f_t = doubles and triples gate fraction,
ν_{sj} = j-th moments of the spontaneous fission neutron distribution,
ν_{ij} = j-th moments of the induced fission neutron distribution.

The gate fractions f_d, f_t represent the proportion of the doubles and triples coincidence signal (respectively) which is observable within the fixed, finite duration coincidence counting interval. Reference [45] gives a description of the calculation of these parameters.

The nuclear data appearing in the point model equations above are the first, second and third reduced factorial moments of the multiplicity distributions. They are defined as:

$$\upsilon_{rj} = \sum_{\nu=0}^{\infty}\frac{\nu!}{j!\left(\nu-j\right)!}P_r(\nu) \quad \text{Eq 4}$$

where r is the reaction identification having value s (spontaneous fission) or i (induced fission) and $P_r(\nu)$ is the multiplicity distribution (probability that in a fission event ν secondary neutrons are generated). To compute them it is therefore necessary to know the multiplicity distributions for spontaneous and neutron induced fission. The knowledge of other nuclear data is necessary, even if they do not appear directly into the equations. To relate the spontaneous fission rate (F) to the ^{240}Pu equivalent mass we need to know the specific spontaneous fission neutron emission rate (neutrons per second gram of Pu), which is determined by the decay constant, the spontaneous fission branching ratio and ν_{s1} of ^{240}Pu. Then to compute the total plutonium mass (^{total}Pu) from the ^{240}Pu effective mass, the same data for the other even numbered plutonium isotopes (^{238}Pu and ^{242}Pu) are used. Moreover to determine the α ratio we need to know the specific (α,n) neutron yields for all the five plutonium isotopes and for ^{241}Am.

In the notation used by LANL and Canberra, one defines the second factorial moment as v2=<v(v-1)> =sum{v(v-1)P(v) taken over v=1 to v_max} and the third factorial moment as v3=<v(v-1)(v-2)>=sum{ v(v-1)(v-2)P(v) taken over v=2 to v_max}. Working in terms of these factorial moments and in the equations for S, D and T one would therefore use v1/1=v1/1!, v2/2 =v2/2! and v3/6 = v3/3! explicitly where vn/n! is called the *reduced* factorial moment. However, in the alternative notation used by JRC (and expressed in equations 1, 2, 3 and 4 above) one works in terms of reduced factorial moments directly such that ν_{sj} denotes the j-th *reduced* factorial moments (that is, the JRC formalism). This may appear confusing at first. However it is simply a matter of convention; the nuclear data and equations are identical. The outcome is that with the (JRC notation) vn in equations 1, 2, 3 and 4 it is necessary to replace these terms by vn/n! to convert to LANL notation. Similarly, it is necessary to replace the terms by n! vn when converting from LANL to JRC formalism.

Expressions for the solution of equations 1, 2 and 3 for the three commonly unknown parameters F, ε and M, are given in references [44] and [46].

4.5.2.2. Nuclear data for neutron transport

In Monte Carlo simulation the entire instrumental device is described and all the possible physical events from neutron generation, during transport, until detection must be adequately modelled. This means that the nuclear data set required is omnicomprehensive. Here we give a short list of physical properties involved:

- cross sections for all neutron reactions for all the materials contained in the samples, sample containers and neutron detectors;
- spontaneous fission data (half-life, branching ratio, neutron yield, multiplicity distributions, secondary neutron spectra) for even isotopes of Pu, ^{238}U and ^{252}Cf;
- induced fission data (neutron yield, multiplicity distributions, secondary neutron spectra, dependence from incident neutron energy) for all U and Pu isotopes;
- (α-n) reaction data (alpha-decay constant, neutron yield in different compounds and emitted neutron spectra) for all U and Pu isotopes and ^{241}Am;
- interrogation source data (neutron yield and spectrum) for AmLi and other sources used in active neutron counting.

Most of the neutron counters have polyethylene as moderator. At thermal energies lattice effects on neutron scattering are not negligible. MCNP can use a special thermal treatment, S(α,β) [4], to model this effect. Unfortunately only a single S(α,β) library is available for polyethylene at 300 K. Extensive studies and the already referred benchmarks have shown some systematic deviations especially in strongly moderated systems. There is also experimental evidence of the influence of temperature. Some improvements in Monte Carlo simulation could be probably expected by a better modelling of the thermal treatment and/or by the production of temperature dependent S(α,β) libraries for polyethylene.

In appendix A we provide a collection of neutron nuclear data that derive from the experience in benchmarking NDA instruments and measurements.

4.5.3. Nuclear data used in gamma spectrometry

The most common application of modelling to gamma spectroscopy in nuclear material safeguards applications is the “physical model” used to interpret the gamma spectra of U and Pu and derive their isotopic composition according to the intrinsic calibration method. This principle finds direct expression in analysis codes such as MGA [47], MGA-U [48] and FRAM [49] and IGA [50].

In practice, the application of Pu and U isotopics analysis codes such as MGA, FRAM and IGA is somewhat different in character, than quantitative codes such as Monte Carlo codes used to calculate detector responses. The codes use nuclear data but this is relative and based on operational experience and may not correspond exactly to book values. Typically only counting statistics are propagated and this is a weakness. In practice, with these codes, issues such as the method of fitting peaks, understanding peak resolution broadening and methods of stripping the spectral continuum, effects of interference peaks, etc, are very important, emphasising the importance of understanding the problem, on commencement of a modelling program.

The nuclear data necessary to perform this type of analysis are those necessary to compute the gamma-ray emissions for the uranium and plutonium isotopes, that reduces to the decay half-lives and the branching ratios, the latter being the probability that following a decay a gamma ray with a specific energy is emitted. There are not a lot of recent and accurate data for branching ratios of uranium and plutonium isotopes, the most complete collection dates back to the 70’s [42].

Nevertheless it is important to remark that when gamma spectrometry is used for isotopic composition determination than for quantitative assessment. This means that it is not required a high accuracy on the absolute values of the individual branching ratios, but a good knowledge of the relative intensities between different energies. This feature has a little bit opened the door to a sort of flexible interpretation of the branching ratios to be used in the gamma spectrometry codes.

Based on the fact that experimentally measured branching ratios are known only with large uncertainties and on the need to have just accurate relative ratios, the branching ratios are often treated not as nuclear data, but as adjustable parameters. This means that often the branching ratio data set has been tuned by the authors in order to reproduce at the best a set of results on experimental data with well-characterised standards. Of course this empirical approach limits the application of the data set of parameter set-up (no longer to be called nuclear data) only to cases contained within the “phase space” of the trial set. Any change of the kind of application to materials or conditions outside the validation boundary will cause a lack of validity of the parameter file and require a new validation or a new parameter set. Of course the adjustment of the branching ratios cannot be left arbitrarily free to the ordinary user. Only the real specialist should be allowed to change the branching ratios and to release a parameter file with a well-defined range of validity and a new appropriate validation.

This empirical procedure has been followed historically in most of the applications of gamma spectrometry to nuclear safeguards and has produced excellent results, so it is considered justified even though for a purist it would seem a little bit "handy craft" and cannot be described as a recommended example of a good practice. From a formal point of view the most correct approach would be as follows. The handycraft probably reflects the fact that the book values need changing. Note also that book values apply across the whole range, but MGA only needs differences in groups:

- to fix the branching ratios and the other nuclear data to the best known available value with their associated uncertainties and store them in a unique configuration file independent from the kind of application;
- for each application domain, benchmarking (see section 4.2) the performances of the system (code + nuclear data) to a set of experimental data;
- to derive accuracy and eventually (application dependent) bias factors;
- to apply "a-posteriori" correction factors to account for systematic deviations of the method.

It should be noted that gamma spectroscopy is also, of course, used for quantitative assay of β/γ isotopes in various applications in waste management and decommissioning, as well as for uranium and plutonium assay in safeguards and waste sentencing. As described above, the validity of any modelling used to calibrate these systems, is dependant on the existence of established benchmarks, covering the full "dynamic range" of the modelling deployed. In applications where calibration relies on computer modelling to calculate the attenuation of gamma rays in a sample (e.g. ISOCS), data libraries describing the mass attenuation coefficient as a function of gamma ray energy, are also used. This data is based upon the photoelectric, Compton scattering, and pair-production cross-sections. The basic principles governing best practice of such libraries, are the same as those described above for neutron cross-sections. The data in these libraries is generally better defined than neutron cross-sections, where there are some known issues for particular isotopes / neutron energies, particularly in regions showing rich resonant structure.

References [34, 35, 36, 37 and 38] provide useful further reading, on this subject.

4.6. Physics treatments

4.6.1. Physics aspects of cross-section data

To a large extent, and especially as far as neutrons and photons of energy below 20 MeV are concerned, the physics involved in Monte Carlo simulation, is fundamentally based on the nuclear data available to and selected by the user. Taking into account effects such coherent/incoherent scattering, form factors, Doppler and temperature effects, angular distributions, the neutron cross-section data is for instance used to determine:

- How far will a particle travel before colliding.
- If a collision occurred, which component isotope was that collision with.
- What fraction of the particle weight was absorbed.
- Which type of reaction occurred.
- How many secondary neutrons are emitted and for each of them what is the energy and angle of emission etc.

There are many data libraries available to users and a serious selection of the library to use for a particular application can thus be important for many reasons.

Neutron cross section libraries, for instance, contain in addition to neutron cross section data for tens of reactions, angular and energy distribution for many reactions, heating numbers, reaction Q-values, photon production cross section etc. These libraries have become so simple to use that they are easy to abuse too. They result from processing the nuclear data evaluations and compilations, which themselves are the fruit of experiments and model codes, using codes such as NJOY to yield data either in a so called pointwise or multigroup form.

In generating data, various evaluation and processing methods are used and many approximations, assumptions and choices are made, such as choice of experiments and representations, interpolation, thresholds, Q-values, representation of angular distributions as equi-probable bins, etc. For the same evaluation, a different processing may also be applied using different processing codes (NJOY, TRANSX, AMPX, SCALE), resulting in either full continuous (class C, e.g. 26000.60C in MCNP jargon), thinned continuous (e.g. 26000.61C in MCNP) or discrete energy data (e.g. 26000.60D), which might also have different temperatures, tolerances etc. Discrete energy versions (Class D) of continuous energy libraries have often been produced, when computer memory was of essence, whereby

all cross sections are averaged into a fixed set of 262 energy bins.

In choosing neutron cross section tables, one should thus consider the sensitivity of results to different evaluations and philosophies, the neutron energy spectra involved, the temperature at which data were processed and the availability of photon-production data. This is achieved by running the modelling codes using cross-section libraries or using special codes designed to produce tailored cross-sections for use by specific modelling codes / applications.

Above 20 MeV and up to 150 MeV, some nuclear data has to some extent become available in recent years but this is still insufficient. Thus, a combination of data, nuclear models and various approximations are often made use of to the best one can. Above 150 MeV theoretical models, with their assumptions and approximations are in general the only option.

Electron transport physics is important in some gamma assay modelling applications, where the secondary gamma radiations produced by electron (photoelectrons) interactions, are important for the particular calculation. In electron transport, the physics primarily based also on the cross section data available to which, more approximations (than for neutron transport) are applied and the effects (e.g. bremsstrahlung) considered are more varied. Various algorithms for multi-scattering are used in electron transport which is analogue in essence. The user must be aware of, not all which cross-section data is used, but also of all the models, algorithms and approximations, assumptions and defaults options (cards) used within a code as to avoid the black box syndrome.

4.6.2. Variance reduction techniques

For problems where analogue simulation is inappropriate, a non-analogue game can be played by sampling from a distorted transport kernel, whereby the expectation values of the different scores are preserved, whilst the particle histories that contribute most to the required scores are forced to be sampled more frequently. Such methods are universally used for deep penetration problems or highly scattering problems [51, 52 and 53].

The objective of distorting the transport kernel (known as biasing) is to reduce either the variance of the score (variance reduction techniques) or the computer “runtime” (acceleration techniques) needed to obtain a given statistical accuracy.

A measure of the success of any biasing method can be obtained by investigating the ratio $\frac{1}{\sigma^2 T}$

where σ^2 is the variance on the final score and T is the computer time used to obtain that variance. This ratio is often called the Figure of Merit (FOM) for the simulation. An increase in the FOM, which depends also on the machine used, indicates an increase in the efficiency with which the simulation is being performed.

Many effective biasing schemes exist are currently being developed further. Some of the methods, such as particle splitting and Russian roulette, have almost universal application, whilst others, such as the exponential transform, are limited to certain classes of problem. Some of these techniques require care, for example angular biasing may not allow for scatter build-up properly.

MCNP, for instance, uses the following four types of variance reduction techniques:

- Truncation methods: time and energy cut-off.
- Population control methods: weight cut-off, geometry or/and energy splitting and Russian roulette, weight window generator.
- Modified sampling methods: implicit capture, general source biasing, forced collisions and exponential transform.
- Partially deterministic methods: point and ring detectors and DXTRAN.

These methods and their application are fully described in the MCNP manual and the sample problem paper for variance reduction in MCNP by Booth [54]. It has been shown that applying appropriately most of the above techniques to a deep penetration problem example in the Booth paper, one reaches convergence within a few minutes compared to estimated years of calculations on a 1990’s PC.

Because variance reduction techniques use non-analogue particle transport with no real tracks involved, it can happen that portions of the physical phase space may not be allowed to contribute to the results. In such cases, one may not be sampling the right problem but rather a totally different one; yet giving all seemingly good results that may be inaccurate by as much 2 to 3 standard deviations. This is called false convergence, which is a major pitfall in variance reduction techniques.

This can not happen in analogue transportation (preferred whenever possible) whereby as one is dealing with real physical tracks and particles, one

can not force too much sampling in one area of importance or direction, thus ensuring that the problem to be modelled contains all the source particles. Despite ever more powerful computers, variance reductions techniques are often required in many deep penetration or high scattering problems. However and fortunately many NDA applications such as detector response calculation would not require variance reductions and acceleration techniques in general. Furthermore codes such as MCNP have now installed statistical packages that if added to user experience and open eyes can avoid help in avoiding such pitfalls.

In a Monte Carlo simulation, the average underlying behaviour of the system is inferred from the sampled behaviour of simulated particle histories by invoking the Central Limit Theorem of mathematical probability on which the techniques is fundamentally based. It is thus only appropriate to mention here that one needs to check that central limit theorem is satisfied.

MCNP has arguably one of the most robust statistical analysis packages of all Monte Carlo codes. In addition to the usual mean and variance, the user is provided with the variance of the variance (VOV), which involves the first four history score moments and represents the error of the error. The tally score probability density function (PDF) is estimated and ten statistical checks are incorporated to avoid false convergence. False convergence is quantitatively characterised by the non-existence of the variance or mean (1^{st} and 2^{nd} moments) and thus the non-satisfaction of the central limit theorem, which is the most fundamental principle in the Monte Carlo method. By inspecting the slope of the tail of the underlying tally score PDF one can estimate the number of moments that exist and hence determine whether the VOV, the variance and even the mean exist. The VOV is more sensitive to large history scores and should decrease as 1/N where N is the number of histories.

Sensitivity to other factors such as sample density, container wall details and moisture content, do not produce Gaussian shaped uncertainties. Therefore special consideration (normally through sensitivity studies) is required to determine the shape of their distributions to allow propagation to calculate the correct TMU. The effect of each parameter variation, on the output, must be carefully studied, sampling results using a known probability distribution to represent the realistic possible range of the parameter (for example Gaussian, rectangular, or triangular distribution). A similar sampling exercise would then be followed to combine the effects of simultaneous variability in different parameters.

4.6.3. Thermal effects and related issues

Thermal neutron transportation is complicated by the fact that neutrons do not see a single nucleus but the entire molecule and because the velocity distribution (Doppler broadening) of the target atoms and molecules in the laboratory frame cannot be neglected. Target nuclei are put in motion by the zero-point motion and non-zero temperature of the material as the neutrons tend to be thermalised to the corresponding energies. Low energy and wavelength neutrons may interact with the lattice spacing of the solid thus creating peak structures in cross sections, each one corresponding to a particular set of crystal planes. Furthermore coherent scattering (interference of scattered waves) add constructively in some directions and destructively in others thus affecting the angular distributions (Bragg scattering). The double differential cross sections are also modified as neutrons can loose or gain energy in discrete amounts.

Temperature effects are difficult to model and can be particularly important if AE/kT is small where A is the atomic weight of target, E the neutron energy, k the Boltzmann coefficient and T is the temperature. Consequently, in many problems where thermalisation (< 4 eV) is involved, the thermal $S(\alpha,\beta)$ tables [4] should be invoked to model the neutron scattering as impacted by the binding of the scattering nucleus in the moderator. In MCNP thermal $S(\alpha,\beta)$ tables are invoked using the MT card to model the neutron scattering as impacted by the binding of the scattering nucleus in the moderator. The isotope scattering data is then overridden if one is in the $S(\alpha,\beta)$ energy range.

When comparing the response functions of various polyethylene moderated detectors used in NDA measurements, the agreement obtained is generally better for cadmium lined detectors (fast or epithermal neutron spectrum) than for fully thermalised assemblies. This may suggest that one may need to refine our use and knowledge for polyethylene, perhaps as far as the $S(\alpha,\beta)$ treatment and temperature effects are concerned. Agreement is also often better for cylindrical assay chambers, than for square chambers, indicating the greater degree of difficulty in accurately modelling the multiple scattering of neutrons in corner regions of the latter geometry (where the effects of any inaccuracies in cross-section data will become more pronounced).

A test example is shown in Table 2 whereby a neutron collar detector installed at a processing plan was modelled with and without the S(α,β) treatment for a magazine full of MOX (Mixed Pu-U) oxide reactor pins [55]. The difference in Reals rates, the best signature for verification, is as much as 7.9%. It is 4.2% for Totals rates.

Collar counter – MCNP modelling method	Calculated quantity	Count rate (s^{-1})	Ratio of result (with / without thermal treatment)
with S(α,β) treatment	Reals	1.1999E+04	7.9%
	Total	3.4423E+05	4.2%
without S(α,β)	Reals	1.3023E+04	
	Totals	3.5948E+05	

Table 2: MCNP calculated Reals and Totals count rates for a Collar (for a MOX fuel pin magazine) counter with and without thermal treatment [55].

4.6.4. Neutron multiplicity distributions

In assessing uncertainty budgets and sensitivity analysis, one must bear in mind that a poor knowledge or inadequate use of the multiplicity distributions can generate large uncertainties.

In some codes, as previously done in MCNP, the number of neutrons generated in a fission event is calculated by sampling only two values:

- Integer(<ν>) with probability = 1 – [<ν> – Int(<ν>)]
- [Int(<ν>) + 1] with probability = [<ν> – Int(<ν>)]

While this is reasonably adequate for reproducing, for a large number of events, the average number of neutrons, <ν>, and its derivatives related to the first moment such as neutron fluences, coincidence rates which are associated with higher moments of the multiplicity distributions are not correctly modelled in sampling the number of fission neutrons. Recent modelling codes have successfully modelled the true multiplicity distributions correctly, however.

4.6.5. Importance of random numbers in Monte Carlo modelling

Monte Carlo simulation also relies heavily on using random (or pseudo-random) number generators. Thus one must ensure that the random number generator used is sound and that any correlations between various calculations that may be due to using the same starting pseudorandom number is removed, as has been shown for example at the National Physical Laboratory [56] investigating the response functions and effective centre of a moderated BF3 counter at various energies and distances from the neutron source. In such cases one should ensure that a different random starting number is chosen randomly to avoid unphysical structures and effects in the distributions and entities studied.

References [4, 51, 52, 53, 54, 55 and 56] provide useful further reading, on this subject.

4.7. Treatment of Uncertainties

In this section we define the different kinds of uncertainties, that are relevant for computer modelling applications in the field of NDA. We describe best practice formalisms for expressing the uncertainties of (modelled) quantities, and how to propagate them to give their contributions towards the total measurement uncertainty of the end result of a measurement, consistent with established practice for NDA measurements (see for example [1]). Illustrations are given with reference to examples of typical modelling applications, including typical sources of uncertainty, and how they are expressed, quantified and propagated. The best practice procedures recommended here are consistent with the industry-recommended guidelines for treatment of uncertainties in NDA measurements, noting that modelling techniques are simply tools used to provide some of the parameters (most commonly the measurement parameter) required to evaluate the result of an NDA measurement (usually fissile mass or nuclide activity).

In the last decade, modelling and simulation have been increasingly used in scientific research and in the analysis and design of engineering systems. Studies have been devoted to the estimation of the total modelling and simulation uncertainty in computational predictions (see references [57 and 58] and the references herein). These studies generally consider different definitions of uncertainty and error than those defined and used for experimental measurements. Commonly one can define the following components: variability, uncertainty and error.

Variability describes the inherent variation associated with the physical system or the environment. It is generally represented as a distributed quantity (e.g. the exact dimension of a manufactured part). Variability is also referred to as stochastic uncertainty, aleatory uncertainty, inherent uncertainty and irreducible uncertainty.

Uncertainty describes the source of nondeterministic behaviour and is sometimes also indicated as epistemic uncertainty and reducible uncertainty. Un-

certainty may be defined as a potential deficiency in the modelling or simulation process that is due to lack of complete knowledge (e.g. due to vagueness, nonspecificity or dissonance). As a consequence, uncertainty may be reduced by increasing the knowledge. Uncertainty typically is represented by modern information theories (e.g fuzzy set theory).

Error is defined as a recognizable deficiency in any phase of the modelling and simulation that is not due to lack of knowledge. Examples of errors are the finite precision arithmetic in a computer, approximations made to simplify the modelling of a physical process, mistakes or blunders made by the analyst. Errors may be acknowledged (recognized, magnitude is known) or unacknowledged (not recognized, but recognizable) The term "*Bias*" is often used to represent the fixed deviation between the true value and the measured value, as a result of such errors or mistakes.

According to these definitions, variability and uncertainty differ from the error by the fact that the first two deal with a level of knowledge that is known (albeit this knowledge may be incomplete), while error deals with knowledge (and therefore a potential bias in the results) that is unknown. Variability and uncertainty will produce stochastic, non-deterministic effects, whereas errors yield a reproducible or deterministic bias in the simulation.

Usually, the term "uncertainty" is used to embrace the above – defined terms "variability" and "uncertainty". At this point, it is important to understand the difference between the commonly used terms "random" and "systematic" uncertainties. A random uncertainty is defined by a distribution of possible values of the parameter, centred about a mean value, usually corresponding to the true value. The nature of the distribution function (e.g. gaussian, rectangular, triangular) is important. A systematic uncertainty represents as fixed bias or "error", such that every measurement is different from the true value, by the same fixed amount. Poisson counting statistics is the most common example of a random uncertainty. This terminology has been largely superseded by the terms "Type A" and "Type B" uncertainties [59]. Type A uncertainties are those that can be evaluated by statistical means, whereas Type B uncertainties must be evaluated by other means. Counting statistics is a common example of a Type A uncertainty, whereas the effect of an uncertain waste matrix, is typically represented by a Type B uncertainty because the uncertainty could be manifested as a fixed bias or "offset".

In the field of NDA measurements / modelling, both types of uncertainty can be important. For example, consider the gamma measurement of drums of waste where drums can be classified according to density. Each nuclide activity measurement will be subject to random counting uncertainties. However, the uncertainty on the final activity may be a function of the drum density. For example, it may be known that a certain waste matrix type / density, always gives the same bias, due to the effect of the physics algorithms being always the same for that type of matrix. In this sense, the observed bias in the end result contains both random and systematic components. Thus when talking about drums of that particular matrix type, we can talk about a systematic uncertainty of say "10 % underestimation", as well as a purely random component due to counting statistics. However, when considering a random population of drums containing different matrices, the distribution of systematic bias can usually be treated as a random distribution. Similar examples are also applicable for the results of computer modelling, applied to NDA applications.

The term "*precision*" is often used to represent the repeatability of an observation, measurement or calculation. In the absence of any bias or systematic error, it is often the case that the mean value converges on the true value, if a large number of observations is made. The term precision is often used to represent random, statistical or "Type A" uncertainties.

The term "*accuracy*" is used to describe the closeness of an observation (measurement or calculation) to the true value. Thus an accurate measurement is one with a low bias and uncertainty.

The term "*Total Measurement Uncertainty*" expresses the total uncertainty associated with a measurement. It includes both the random and systematic components, and requires careful propagation of the individual terms.

Further reading on the expression of uncertainties can be found in references [59, 60, 61, 62, 63, 64, 65, 66, 67 and 68].

This section aims at summarizing the most important sources of variability, uncertainty and error in computer simulations related to non-destructive assay and characterization of special nuclear material. This discussion on uncertainty is equally valid for the use of modelling codes for other NDA applications (i.e. for measuring radionuclides that are not, in themselves, classified as special nuclear material). It is assumed that commercially available and validated codes are used for that purpose.

4.7.1. Estimation of total uncertainty determined by the variability of input

Typical simulation problems that are considered here are: particle transport and interactions (neutrons, photons, electrons…), burnup and depletion computations, criticality calculations. These problems are studied with Monte Carlo codes such as: MCNP, KENO, MCBEND, TRIPOLI, MORSE, EGS4, PENELOPE, MONK, ITS, FLUKA, LAHET, or deterministic discrete ordinates codes such as: ANISN, DOORS, DANTSYS, PARTISN, TWOTRAN, CEPXS/ONELD, or simple gamma ray attenuation codes such as ISOTOPIC, ISOCS, MERCURAD / PASCALYS and GAMMASHIELD.

Most of the physical parameters describing these problems are identifiable as variability e.g. each parameter may be represented by a distribution. The important point here, is the uncertainty knowledge of what is the true value of a parameter, which leads to an uncertainty in the end result of the simulation. The total uncertainty resulting from the variability of different parameters is obtained by the well known uncertainty propagation laws. If the simulation result is represented as a response *F* that, given a set of input parameters β_i and δ_i each with its variability σ_i, defines the output then the variability on a simulation result R can be represented as :

$$R = F(\beta_1,...\beta_n;\delta_1...\delta_n) \qquad \text{Eq 5}$$

$$\sigma^2(R) = \sum_{\beta\delta} \frac{\partial^2 F}{\partial\beta\partial\delta}\sigma(\beta)\sigma(\delta) \qquad \text{Eq 6}$$

Evaluation of the covariance terms requires that the matrix of behaviours is analysed.

Typically advanced Monte Carlo methods use the technique of differential sampling that computes the derivatives of the response with respect to some of the input parameters at the same time as the response are used for that purpose. Differential sampling with respect to material parameters is available in MCNP [4]. In such computations one or more of the parameters is varied between its boundaries and the variation of the result is observed. Since not all parameters are independent of one another it may be necessary to investigate possible correlations. However, for codes where such differential analysis is not available, it is necessary for the user to quantify the individual uncertainties by a comprehensive sensitivity study, exploring the sensitivity of the end result to variability in the parameters for which the true physical value is not known.

Interval mathematics is the simplest way to represent total uncertainty when only the bounds of parameters under concern are available. Each uncertain parameter is described by an interval number.

Another approach is to use *response surface methods* which are used to assess variabilities. The only way to determine the uncertainty will be by using the simulation code itself.

4.7.2. Analysis of different types of uncertainty

Table 3 lists the most important parameters generally used in simulation programs considered in this document.

The physical dimensions:

A problem definition (see section 4.1) for the simulation of particle transport requires that the dimensions of all objects are properly defined. In practice the dimensions are only known with limited accuracy e.g. the dead layer of a HPGe detector crystal, the specific shape of the HPGe crystal when it is bulletized, the effective length of the anode wire in a ^{3}He detector tube etc. In these situations the best estimates should be used for these parameters, and it may be necessary to investigate the impact by considering different values for these parameters. In many situations the actual geometry is simplified, and details (e.g. small objects) which are believed not to be important are not considered in the simulation. Care should also be used in determining where the actual problem ends in space (e.g. it may be necessary to consider reflection by nearby walls that at first sight may appear as not being part of the problem).

Chemical composition:

It is the properties of the materials that build the problem geometry that will determine the transport of particles and their interactions with these materials. Depending on the values of the cross sections for certain interactions some elements or isotopes may have an important impact on the result. Hence the material compositions should be considered with care, and laboratory analysis may be required to determine the actual composition of certain materials in the problem. Moreover in some problems, attention should be even paid to trace elements or impurities that may exist in the materials. If these impurities have large interaction probability with the particles considered (e.g. neutron poisons) neglecting these may result in strongly biased results.

Material density:

The density of materials together with the composition determines the reaction rates of the particles

that will interact with the material. The density of materials is often looked up in standard tables describing the physical properties of materials, however in practice the actual density may deviate from these values and it may be required to determine the density (e.g. the density of polyethylene used as neutron moderator). For gas filled detectors it is very important to know precisely the gas pressure and eventually to correct for temperature in order to determine the number of atoms per unit volume. The density and composition of any gamma shields / collimators (especially graduated filters) is obviously important.

Nuclear data:

Cross sections are generally part of the simulation code and the user may not have to provide these. However in some simulation codes the user may select the cross section libraries. Cross sections should be selected with care and with judgment expertise: the libraries should be fit for purpose e.g. the temperature at which cross sections are given should correspond to the considered temperature in the problem, when considering discrete energy groups, the grouping should be apt for the problem considered.

For gamma calculations, the half-lives and gamma attenuation cross-section libraries are relevant. The branching ratios and abundances of gamma emissions are important for quantitative gamma spectroscopy calculations, while knowledge of the neutron yields and multiplicity data is critical to understanding the uncertainties for neutron counting modelling. Calculations performed with different credible data sets may be used to estimate the state of knowledge uncertainty.

Monte Carlo calculation statistics:

In Monte Carlo simulation, one of the most important computational parameters is the number of initial particles that is run. Most codes consider the influence of this parameter and report results together with a relative uncertainty due to the finite number of histories that were run. This uncertainty however may not be considered as the total uncertainty. Consideration should also be given to the statistical convergence of a tally, as the number of source particles increases. Some codes, for example MCNP [4], provide tools for monitoring this convergence. If tallies are “well behaved”, then the standard deviation will be inversely proportional to the square root of the number of source particles that have been tracked. However, it is possible that rare events (for example occasional contribution from very high weight particles) can give large step changes in tallies, causing departure from this normal behaviour. Most Monte Carlo codes automatically provide statistical uncertainties as part of the normal output, so this component is easy to assess. Tally fluctuation charts should be inspected to check for such behaviour, with reference to the guidelines in the code manual (for example, [4]).

When using physics – based “variance reduction” techniques to “accelerate” Monte Carlo runs, effectively increasing the number of source particles that are tracked, great care must be taken to ensure that correct procedures are followed in accordance with the recommendations of the code authors and established benchmarks, in order to ensure that the results are reliable, and that no significant bias (systematic error or unacknowledged error) is apparent (see section 4.6 for further discussions on this subject). Techniques appropriate for one type of problem (for example uncollided flux) may not be suitable for some other types of problems (for example where scatter contribution is needed).

Possible sources of error or bias:

Sources of error, as defined above, may be identified at two distinct levels: errors induced by the user of the code (e.g. simplifications used to describe the problem with the input parameters) and errors inherent to the code (e.g. made by the developers of the code).

Acknowledged errors:

Acknowledged errors are known by the modeller and the magnitude (bias) may be investigated. Some examples of typical acknowledged errors are given in the Table 4.

Unacknowledged errors:

Unacknowledged errors by definition are not accounted for when considering total uncertainty. As such, unacknowledged errors are mistakes, which are best avoided by thorough verification. Examples of unacknowledged errors are given in Table 5.

4.7.3. Total uncertainty in absolute versus relative simulations

Simulations results generally can be used in two ways: as an absolute simulation result (e.g. absolute detection efficiency of a HPGe detector) or in a relative way where the actual result is the ratio of two simulation results. Relative simulation results are typically used to predict a response of a measurement situation which is not too much different from another measurement situation (e.g. detector response of a point source compared to a small volume source in gamma ray spectrometry).

Parameters subject to variability
Physical dimensions of objects
• Active length of detectors (e.g. anode wire length in the case of 3He detectors)
• Dimensions of sample container
• Dimensions of chamber walls
• Germanium detector dimensions, dead layer details, inner core geometry and bulletisation.
Chemical composition of sample
• Enrichment
• Isotopic composition
• Trace elements, impurities
• Neutron absorbers
• Fissile material
• Compound
Density of materials
• Physical state
• Apparent density
• Distribution of material
• Gas pressure (e.g. 3He proportional counters)
• Density / voidage of the structural materials used to construct a measurement chamber (e.g. polyethylene)
• Density of gamma shields / collimators
• Elemental composition and density of sample “matrix”
Nuclear data
• Origin of library
• Discrete or continuous cross-sections
• Types considered
• Half-lives
• Gamma attenuation data
• Temperature at which cross sections are evaluated
• Neutron source spectrum
• Neutron source isotropy
Irradiation/cooling history
• For example the uncertainty in the fixed ratio between the activity of an inferred nuclide and one that is directly measured.
Stochastic uncertainties from Monte Carlo modelling
• Statistical uncertainty associated with the Monte Carlo result or “tally”, due to the simulation of a finite number of particles in a “run”

Table 3: Important parameters generally used in simulation programs, for which the uncertainty should be considered.

Acknowledged error
Cut of parameters used in a Monte Carlo code
• Energy cut-off
• Particle weight cut-off
Effect of Boundary conditions
• Reflecting walls
Effect of Boundary conditions
• Reflecting walls
• Absorbing walls
Discretization
• Spatial step sizes and grids
• Discrete angular direction quadrature set (anisotropy)
• Temporal step sizes
• Conversion from continuum mathematics to discrete mathematics (binning)

Table 4: Examples of acknowledged errors in application of modelling codes.

Computation parameter
Mistakes in the input:
Incorrect cross-sections used
Incorrect use of physics techniques such as the following, leading to a bias in the results:
Mis-use of variance reduction techniques
Mis-use of physics approximations (e.g. importance functions, treatment of electron scattering)

Table 5: Examples of unacknowledged errors in application of modelling codes.

The absolute simulation clearly will by the most sensitive to the variability of the input parameters and errors.

When considering the ratio between two problems that are not too different from one another, the impact of certain problem definition parameters can be minimized. It is usual to perform such relative calculations, within the confines of a known parameter space for which benchmark data exists, and so the results are known to be reliable.

4.7.4. Expression and propagation of uncertainties

It is important to ensure that each result of a modelling simulation is expressed together with its associated uncertainty, in a manner which both ensures clarity (that is, it is clear to the end – user exactly what the result means) and facilitates straightforward propagation of uncertainties so that the impact on the uncertainty on the final NDA measurement result can be calculated.

The recommended basic steps to follow in the evaluation and expression of uncertainties associated with modelled parameters which relate to a measurement quantity through calibration, are as follows:

1. Identify the key input uncertainties with respect to their different outputs.
2. Identify different possible model formulations and compare them.
3. Identify the nature of the various parameter uncertainties (e.g. random versus systematic uncertainties).
4. Obtain estimates for the uncertainty associated with each of the input parameters which are fed into the modelling process.

5. Determine the effect of each input uncertainty on the associated uncertainty in output quantity (for example, a detector tally).

   Sensitivity studies are often used to determine the effect of an uncertain input parameter, on the uncertainty associated with the output parameter.

6. Determine the standard uncertainty for each parameter.

7. Propagate the standard uncertainties on the individual model parameters, to determine the effect on the instrument calibration parameter and ultimately the standard uncertainty on the final measurement quantity.

8. Apply the appropriate multiplier to express the final result at the desired confidence level.

We present below, a formalism for expressing and propagating uncertainties, based on established practices [1, 59 and 61].

The expression of the value of the result of a measurement or calculation, F, is incomplete without a statement of its evaluated uncertainty, *U*. This characterises the range in which the "true value" is estimated to lie with a given level of confidence. Any particular observation (i.e. measurement or calculation) will then produce a sample value that lies somewhere within a defined probability distribution function at which the "true value" is usually located at the mod-point (for example in a Gaussian or "normal" distribution). It is important to understand the nature of the probability distribution function, because it is usually the confidence level that is of direct interest to the end-user.

Each parameter has an associated uncertainty σ_i that characterizes the spread of values within which the true value x_i is believed to lie. If x_i may lie anywhere within a specified range of values with equal probability, it is said to have a rectangular probability distribution and the uncertainty is expressed in terms of the value for the semi-range. Alternatively, the probability distribution can be normal (i.e. Gaussian), and the standard deviation (or a given multiple of the standard deviation) may be used. An uncertainty should always be expressed in terms of a numerical value for an associated level of confidence. This obviously means that the type of the probability distribution should also be known. If the nature of a particular distribution is unknown, a conservative approach is to assume that it is a rectangular distribution, as this will lead to a conservatively high standard uncertainty value.

Table 6 summarises the common types of probability distribution functions that are relevant when calculating uncertainties. The "divisor" gives the number by which the stated uncertainty parameter must be divided, to give the corresponding "standard uncertainty" at a 67.7 % confidence level, equivalent to "one standard deviation". When propagating uncertainties, one should use the standard uncertainty value for each parameter.

The combined standard uncertainty of the output quantity, *u*, is derived by the summation in quadrature of each of the individual standard uncertainty terms as shown in equation 7 (assuming that the terms are uncorrelated).

$$u = [\Sigma u(\beta_i)^2]^{1/2} \quad \text{Eq 7}$$

Guidance for procedures to propagate uncertainties can be found in the literature [62, 63, 64, 65, 66, 67 and 68].

Distribution	Parameter	Confidence level	Divisor (k)
Normal	1 standard deviation	67.7%	1.0
Normal	2 standard deviations	95.5%	2.0
Normal	3 standard deviations	99.7%	3.0
Rectangular	semi-range	100%	√3

Table 6: Common types of probability distribution functions.

The above expression applies only when the input quantities are independent of each other, i.e. when they are uncorrelated. Correlation analysis [61] should be used if this assumption does not hold. Furthermore, care may be required to allow for the non-normal behaviour of the "high end tail" of common probability distributions.

When the standard uncertainty has been calculated, after propagating each of the individual terms, an appropriate multiplier or "coverage factor" should be applied so that the final uncertainty result is expressed at the desired confidence level. The standard uncertainty (multiplier of 1) equates to a confidence level of 67.7 %. If a multiplier of 2 is applied (equivalent to 2 standard deviations for a normal distribution) then the confidence level is 95.5 %. Similarly, a multiplier of 3 gives a confidence level of 99.7 %. It is common, in NDA applications, to adopt a 95.5 % confidence level (multiplier of 2). A similar concept is applied as a coverage factor is needed to adjust the standard deviation for a small sample to represent a given confidence level for an infinite number of degrees of freedom (that is, the "students t distribution").

It is usual to provide an uncertainty budget, so that the individual terms are identified, together with their relative importance. As an example of a typical real – life application, consider the following example whereby MCNP modelling has been used to calibrate a Passive neutron Coincidence Counter (PNCC) for Pu assay of waste-bearing containers. This example shows how the uncertainties associated with the individual parameters are evaluated, and propagated through the instrument calibration to show the effect on a final measurement result. Table 7 shows how the individual uncertainty components are expressed, identified, and propagated.

In this example, MCNP is used to apply a "relative" calibration for a particular waste container / matrix geometry, for which it is not possible to perform a direct measurement using standards. Calibration measurements have been performed using Pu standards at the centre of an empty drum, and MCNP modelling is used to allow for the effects of the specific waste matrix, and to allow for the known spatially uniform Pu distribution within the container. It is assumed that an appropriate benchmark exists to illustrate the performance of MCNP modelling, when compared with results of experiments, for which the geometry details are accurately known (that is, there are no additional MCNP uncertainties as a result of uncertain system geometry, for these benchmark systems).

Item 1 relates to the statistical quality of the MCNP – calculated efficiency result, while the uncertainty for item 2 (the "Coincidence Reals" response) is simply obtained by squaring the uncertainty on item 1, since the Reals response is proportional to the square of the detection efficiency. Item 3 relates to the known variability observed for representative benchmark experiments with a simple reference geometry such as an empty drum. In stating a rectangular distribution, we are assuming that the measurement / MCNP discrepancy lies within a defined range, with an equal probability across the range. This method of dealing with benchmark uncertainty applies to cases where

Item	Parameter	Symbol	Uncertainty	Probability distribution	Divisor	u_i (± %)
1	Statistical uncertainty associated with MCNP – calculated efficiency tally	β_1	1 %	Normal	1	1
2	Statistical uncertainty associated with "Coincidence Reals" calibration parameter	β_2	2 % [= 2 β_1]	Normal	1	2
3	Known uncertainty due to benchmark experiment performance for empty drum, with accurately modeled geometries	β_3	15 % (semi-range)	Rectangular	√3	9
4	Uncertainty associated with MCNP – calculated matrix perturbation	β_4	20 (semi-range)	Rectangular	√3	12
5	Geometry model approximation uncertainties (detector active length, polythene density, etc)	β_5	5	Gaussian	1	5
6	Physics uncertainties (neutron source spectrum, neutron cross-sections, neutron multiplicity second factorial moments)	β_6	0	N/A	N/A	0
	Propagated standard uncertainty on MCNP – calculated calibration parameter = $(\Sigma\ (i=1\text{-}6)\ u_i^2)^{0.5}$	β_{MCNP}	N/A	Gaussian	N/A	16
7	Propagated standard uncertainty on measured calibration response parameter for Pu standards	β_7	10	Gaussian	1	10
	Expanded standard uncertainty on final calibration parameter = $(\beta_{MCNP}^2 + \beta_{CALIB}^2)^{0.5}$	β_{CALIB}	N/A	Normal	N/A	19
	Expanded uncertainty at 95.5 % confidence level	U	N/A	Normal	2	38

Table 7: Example uncertainty propagation: PNCC assay of Pu in waste loaded drums.

no benchmark exists for the as-built chamber. Alternatively, it is sometimes possible to establish a benchmark for the as-build system, in which case a simple correction factor is applied to take account of the known measurement – modelled result bias. Similarly, item 4 refers to the use of MCNP to calculate the perturbation effect of a defined matrix. Item 5 refers to uncertainties due to the fact that the exact details of the assay chamber are usually not known. Any additional uncertainties (item 6) from physics approximations and nuclear data, are neglected because in this example it is assumed that the same nuclear data is used, as for the benchmark systems (see item 3). The effects of uncertain nuclear data and physics approximations are therefore already included in the uncertainty for item 3.

We see that the propagated standard uncertainty for the modelled response is 16 %, and in this case the individual terms have been added in quadrature because the individual items are multiplicative with regard to their contribution to the final calibration parameter. In this example the standard uncertainty on the measured calibration parameter, which equates to the count rate per unit mass of ^{240}Pu effective at the centre of an empty drum, is 10 %. The final calibration parameter (count rate per unit mass of ^{240}Pu effective distributed uniformly throughout the matrix-loaded container) is therefore given by the product of the measured calibration parameter and the MCNP-calculated response expressed as a ratio to the empty drum “centre” position. This leads to a final uncertainty of 19 % at 67.7 % confidence, or 38 % at 95.5 % confidence (that is, a multiplier of 2).

In the above example, we have presented a simplified problem, in the sense that we have assumed each input parameter to be independent. For more complex problems, it may be necessary to fold the individual probability density functions (PDF’s).

Further reading may be found in references [59, 60, 61, 62 and 63].

It is important to note that for real NDA applications it is not only the modelled parameters that must be taken into account when determining the uncertainty on a measured quantity. In practice there are various other factors which are not amenable to assessment using the techniques described in this guide, such as the following. These required careful consideration by experimentation.

- Effects of pulse pile-up leading to loss of peak resolution.
- Deadtime losses.
- Interference (to a gamma peak of interest) from other species (for example performing Pu isotopics measurements in the presence of a high gamma background from fission products).
- A bias may occur if assumptions that are made as part of the calibration, are not true (for example a sample is not, in practice, in true secular equilibrium).
- Electrical noise.
- Temperature effects (drift) in the detector and amplifier.
- Dead layer growth (in Germanium detectors) which may alter the efficiency and invalidate the calibration.
- Physical changes such as moisture content, temperature, air pressure and humidity, seasonal neutron background variations, people moving in the vicinity of neutron counters (changing the moderation), etc.

5. Conclusions

The use of computer-based modelling tools is becoming increasingly widespread in the support of Non Destructive Assay (NDA) measurements, both in the context of development of the techniques, and calibration of measurement equipment. The increasing availability of powerful computing systems is making this possible, whilst the availability of calibrated nuclear material standards is diminishing. For these reasons, increasing reliance is being placed on the modelling tools. This means that it is becoming increasingly important to be able to demonstrate the validity of the results of modelling techniques, both to internal stakeholders and to regulators.

The specialist nature of the codes considered in this report (Monte Carlo codes such as MCNP, MCBEND, KENO, Reactor Physics depletion codes such as FISPIN, ORIGEN, and ray-tracing analytical codes such as ISOCS and ISOTOPIC) generally means that expert and experienced physicists are required to run the codes and interpret the results. This highlights the importance of training and development / implementation of Quality Assurance procedures, to ensure that the codes are operated correctly, and within the known and documented operational range for the codes. However, the technical issues are complex, and require careful consideration to assess validity of modelling calculations.

This report considers each of the issues that must be considered to ensure reliable use of modelling codes in the field of NDA. Both technical (physics,

nuclear data, benchmarking, uncertainties, etc) and management (QA, training, etc) issues are considered. We illustrate, through worked examples of real-life applications, how modelling codes are successfully used to calibrate NDA measurement systems. This leads to identification of the key issues that determine the reliability and accuracy of modelling results, and suggestions for further work. We have shown how the correct use of modelling codes can lead to highly accurate calibrations of NDA systems without relying on the use of physical standards, provided that sound training and QA principles are followed, and that strict benchmarking is followed. Benchmarking consists of ensuring the reliable performance of the modelling technique within a parameter space for which reliable validations (comparing a measured with a modelled result) exist. We have also shown the importance of a rigorous treatment of uncertainties, when assessing the results of computer modelling, and presented a formalism, consistent with established best practice for NDA measurements, for both expressing the modelling results and propagating the individual terms to show the impact on the final NDA measurement result.

It is concluded that the ultimate limit to the accuracy to which modelling codes can be used to predict NDA system responses (which are not challenged by count rate and environmental factors), is determined by the accuracy of the nuclear data which is used by the codes (for example half-lives, stopping powers, neutron spectra, neutron multiplicity data) and any subsequent interpretational models. This limits the accuracy with which codes can be used to make absolute predictions of count rates / system calibrations. However, when applied for relative calculations, provided that comprehensive and valid benchmarks are used to establish the predicted / measured response ratio, these biases can be removed through normalisation. There are many published benchmarks, however work is required in the NDA industry to maintain good benchmarks as NDA measurement techniques are being applied for more diverse nuclear material fuel types. A good example of this is the use of Monte Carlo modelling techniques to calibrate neutron counting equipment for safeguards measurements of fissile material. Whilst at the present time the known nuclear data, used in combination with benchmark experiments, is sufficient, this will not necessarily be the case when new more exotic fuel types are becoming subjected to safeguards measurements. For these reasons, a high degree of emphasis should be placed on the continual evaluation and improvement of nuclear data.

In this report we describe each of the best practice topics highlighting the principles which if followed, will ensure reliable modelling results. It is hoped that this will be a useful guide for both modelling practitioners and other stakeholders including management, regulators, and “intelligent customers”.

6. Glossary

The following terms are used in this document:

Analytical codes – Codes which use analytical techniques to model a radiation transport problem, based on using equations to model the effects of the sample material on the radiation transport.

Benchmarking – Measurements or experimental tests carried out under reference conditions to produce results against which the results of measurements or tests carried out under other conditions may be compared.

Systematic Bias – A deviation that produces a consistent (repeatable) deviation from the true value in a given situation.

Burn-Up codes – See *Reactor Physics Codes*

Calibration – Procedure to establish a quantitative relation between the response of an instrument and the quantity to be measured. Performed by using analytical techniques, measurements or computer modeling involving one or more reference standards and / or validated computer codes and interpretational models, under a set of reference conditions.

Calibration Factor – Reciprocal of response. Factor by which a reading is multiplied to obtain the quantity being measured.

Central Limit Theorem – A statistical theorem which states that the sampling distribution curve that results from combining many independent variates will be centered on the population parameter value and it will have all the properties of a normal distribution.

Confidence Level – A number expressing the degree of confidence in the result; usually expressed as confidence band in terms of a percentage or as a number of standard deviations.

Coverage Factor – A number that is multiplied by the combined standard uncertainty to give an expanded uncertainty for a given confidence level.

Depletion Codes – See *Reactor Physics Codes*

Error – A deviation from the true value, normally brought about as a result of an incorrect or uncertain calculation or interpretation of a measurement.

Expanded Uncertainty – The standard uncertainty (or combined standard uncertainty) multiplied by a coverage factor for a given confidence level.

Gamma Spectrometry – A radiological assay technique involving the identification and quantification of b/g radionuclides by analysis of the pulse height distribution (spectrum) recorded in a detector.

Hard modeling application – Sometimes also referred to as *Absolute*. Refers to application of modeling tools where the modeling is used to directly calculate a result, without recourse to normalization against any measurement result.

Interpretational Model – An algorithm embodying a set of equations and approximations / assumptions, that is used to convert calculated or measured individual parameters, into a directly measurable response parameter.

Matrix – The material surrounding or holding the substance being assayed. This material may significantly affect the response of the system by attenuation, absorption and other effects on radiation emerging from or entering the substance.

Measurand – A directly measured quantity.

Monte Carlo – A family of computer modeling codes that directly simulates the behaviour or particles by modeling the physical scattering / absorption behaviour, to predict the results of measurable quantities.

Non-Destructive Assay – The observation of spontaneous or stimulated (induced) radioactive emissions, interpreted to estimate the amount of one or more nuclides of interest in the item being assayed, without affecting the physical or chemical form of the material, and without opening the container.

Passive Neutron Coincidence Counting – A technique that counts bursts of neutrons, for example as time-correlated pairs, usually deployed in Non Destructive Assay to quantify Pu.

Passive Neutron Multiplicity Counting – A variant of Passive Neutron Coincidence Counting in which data on the number of neutrons detected together in a burst, is retained.

Precision – A measure of the reproducibility of a measurement / calculation result comprising contributions from repeatability of the measurement / calculation and random counting / modeling statistics.

Random uncertainty – The uncertainty for a parameter for which an individual measured value lies within a distribution that contains the expectation value formed over repeat measurements (Type A uncertainty).

Reals – The directly measured output quantity of a passive neutron coincidence counter based on shift register time analysis.

Reactor Physics Codes – Commonly also referred to as “Burn-up codes”, “Depletion codes” or “inventory codes”. Used to simulate the behaviour of materials in a reactor environment, and calculate the resulting inventory of radionuclides in the fuel / other reactor components.

Reference Standard – A physically and chemically stable item for which the attributes of interest are well-characterised and traceable to primary standards, and for which the other properties affecting the measurement technique are known. Reference standards are used in a measurement system to establish the relationship between the basic instrument response and the attribute(s) of interest

Repeatability – Intrinsic instrument variability – a measure of the agreement between repeated measurements of the same quantity under unchanged conditions of measurement.

Reproducibility – A measure of the agreement between repeated measurements of the same quantity under changed but replicated conditions of measurement.

Response – The ratio of the observed reading of an instrument to the true value of the quantity producing that reading.

Soft modeling application – Sometimes also referred to as *Relative*. Refers to application of modeling tools where the modeling is used to infer the result by taking ratios against directly measured quantities.

Standard Deviation – The positive square root of the variance.

Standard Uncertainty – Uncertainty of a measurement expressed as a margin equivalent to plus or minus one standard deviation.

Stochastic – Description of a process whereby the value is subject to inherent random variability.

Systematic uncertainty – An uncertainty that is represented by a constant bias or off-set, for a measured value compared to the true value under a given condition.

Total Measurement Uncertainty – A combination of the evaluated precision and bias terms, to express the total uncertainty on a measurement or calculation result. The Total Measurement Uncer-

tainty is normally expressed at a defined confidence level, commonly at 95 %.

Traceability – The ability to relate measurements to appropriate national or international standards through an unbroken chain of calibrations carried out in a technically sound manner.

Type A uncertainty – An uncertainty that can be evaluated using statistical means, from replicate measurements.

Type B uncertainty – An uncertainty that must be evaluated using non-statistical means.

Uncertainty – Parameter, associated with the result of a measurement, which characterises the dispersion of the values that could reasonably be attributed to the quantity being measured.

Variability – The inherent variation associated with the measurement / calculation system and its environment. Also refers to stochastic variations.

Variance – A term used to describe the dispersion of a set of observations with respect to its arithmetic mean. Equal to the mean square deviation from the arithmetic mean.

The following acronyms and symbols appear in this document:

α – Ratio of random-to-spontaneous fission neutron production rates for non-multiplying plutonium bearing material

AWCC – Active Well Coincidence Counting: a neutron technique based on discriminating between neutrons from fission induced by an external source and the interrogating radiation (random neutrons). Sometimes known as ANCC (Active Neutron Coincidence counting)

BWR – Boiling Water Reactor

CPU – Central Processing Unit

DG-TREN – Euratom Safeguards Inspection department:

– Directorate General for Transport and Energy

DXTRAN – A technical term used in relation to a specific type of variance reduction featured within the MCNP code.

ENDF – Evaluated Nuclear Data File

$\mathbf{E}$ – Efficiency of detector system

FOM – Figure Of Merit

HEU – Highly Enriched Uranium (normally meaning having a ^{235}U proportion greater than 20 %).

HPGe – High Purity Germanium used for gamma-ray detection and energy measurement

IAEA – International Atomic Energy Agency

JEFF – Joint Evaluated Fission and Fusion File

JENDL – Joint Evaluated Nuclear Data Library

ILW – Intermediate Level Waste

FDET – Fork Detector Irradiated Fuel Measuring System

FORK – Safeguards detector used for spent fuel burnup measurement

JRC – Joint Research Centre

LLD – Lower Limit of Detection

LLW – Low Level Waste

LWR – Light Water Reactor

m_{eff} – Effective ^{240}Pu mass of plutonium (or other nuclear material)

M_L – Neutron leakage multiplication

MOX – Mixed (plutonium and uranium) Oxide – a reactor fuel type

NaI(Tl) or NaI – Thallium-activated sodium iodide (a scintillator material used for gamma-ray detection and energy measurement)

NDA – Non Destructive Assay

NMA – Nuclear Material Accountancy

PDF – Probability Density Function

PERLA – "Performance Laboratory" at Joint Research Centre (JRC) / Ispra

PNCC – Passive Neutron Coincidence Counting: a neutron technique based on discriminating between time-correlated neutrons from spontaneous fission materials and single neutrons from other sources

PNMC – Passive Neutron Multiplicity Counting: a neutron technique based on the measurement of singles, double coincidences and triple coincidences of neutrons emitted from sample

PWR – Pressurised Water Reactor

$^{240}Pu_{eq}$ or $^{240}Pu_{eff}$ – ^{240}Pu equivalent mass (or ^{240}Pu effective mass)

R&D – Research and Development

SF – Spontaneous fission

SNF – Spent Nuclear Fuel

SNM – Special Nuclear Material

$^{total}Pu$, ^{tot}Pu or Pu^{total} – Total plutonium mass

TMU – Total Measurement Uncertainty

VLRM – Very Low level Radioactive Material

VOV – Variance Of the Variance (a term used in statistical analysis of Monte Carlo modeling results)

VVER – "Voda-Vodyanoi Energetichesky Reaktor" (Russian equivalent for PWR reactor)

The following established modeling and data analysis codes are cited in this document.

AMPX – Nuclear data / processing code

ANISN – Discrete ordinates radiation transport code

CEPXS – Discrete ordinates radiation transport code

CESAR – Reactor Physics code

DANTSYS – Discrete ordinates radiation transport code

DOORS – Discrete ordinates radiation transport code

DORT – Discrete ordinates radiation transport code

EGS4 – Monte Carlo code

FISPIN – Reactor Physics code

FLUKA – Monte Carlo code

FRAM – Gamma ray analysis code for plutonium and uranium isotopics assay

GAMMASHIELD – Software for calculating gamma ray attenuation

IGA – Software for the determination of actinides isotopics

ISOCS – Software for calculating gamma ray attenuation and gamma detector efficiencies

ISOTOPIC – Software for calculating gamma ray attenuation

ITS – Monte Carlo code

KENO – Monte Carlo code (used for criticality calculations)

LAHET – Monte Carlo code

MCBEND – Monte Carlo code

MCNP – Monte Carlo code

MCNP-PTA – Variant of MCNP used for simulating neutron pulse trains

MCNP-REN – Variant of MCNP used for simulating NDA counting systems

MCNP-VISED – Visualisation software for MCNP

MERCURE – A dose-rate modelling program.

– Version 6 is distributed by Canberra through the MERCURAD human graphical interface.

MGA – Gamma ray analysis code used to determine plutonium isotopics

MGA-U – Gamma ray analysis code used to determine uranium isotopics

MONK – Monte Carlo code

MORSE – Monte Carlo code

NJOY – Nuclear data / processing code

ORIGEN – Reactor Physics code

PARTISN – Discrete ordinates radiation transport code

SCALE – Nuclear data / processing code

SOURCES – Nuclear data / processing code

TORT – Discrete ordinates radiation transport code

TRANSX – Nuclear data / processing code

TRIPOLI – Monte Carlo code

TWOTRAN – Discrete ordinates radiation transport code

References

[1] P. McClelland and V. Lewis (Ed). National Physical Laboratory Measurement Good Practice Guide No. 34. Radiometric Non-Destructive Assay. ISSN 1368-6550, January 2003.

[2] Numerical Modelling Concepts for IAEA Safeguards. Report of the Co-ordinated Technical Meeting, IAEA, Vienna, 19-21 December 2006.

[3] R. Venkataraman,, M. Villani, S. Croft, P. McClay, R. McElroy, S. Kane, W. Mueller, R. Estep. "An integrated Tomographic Gamma Scanning system for non-destructive assay of radioactive waste", Nucl. Inst. Meth. in Phys. Res. A 579 (2007), 375-379.

[4] MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, LA-UR 03 1987, LA-UR 093,0425.

[5] R. Venkataraman, F. Bronson, V. Atrashkevich, B.M. Young, and M. Field. (Canberra Industries, Meriden, CT., USA). "Validation of In-Situ Object Counting System (ISOCS) mathematical efficiency calibration software." Presented at the Ninth Symposium on Radiation Measurements and Applications, May 11-14, 1998 Ann Arbor, MI, USA. Also published: Nuclear Instruments and Methods in Physics Research (A), 422 (1999), pp. 450-454.

[6] R. Venkataraman, F. Bronson, V. Atrashkevich, M. Field, and B.M. Young. "Improved Detector Response Characterization Method in ISOCS and LabSOCS", Journal of Radioanalytical and Nuclear Chemistry, Vol. 264, No. 1 (2005), 213-219

[7] W.F. Mueller, F. Bronson, M. Field, K. Morris, D. Nakazawa, R. Venkataraman, and V. Atrashkevitch. "Challenges and techniques to effectively characterize the efficiency of broad-ener-

gy germanium detectors at energies less than 45 keV", Paper presented at MARC-VIII (Methods and Applications of Radioanalytical Chemistry) conference, Hawaii, April 6-10, 2009, Accepted for publication in the Journal of Radioanalytical and Nuclear Chemistry (2009)

[8] MCBEND: A Monte Carlo program for general radiation transport solutions, ANSWERS/MCBEND (94) 15, Answers software service, Serco Assurance.

[9] J.P. Both, H. Derriennic, B. Morillon and J.C. Nimal. "A survey of TRIPOLI-4", Proceedings of the 8th International conference on Radiation Shielding, Arlington, Texas, April 24-28, 1994, pp 373-377.

[10] GEANT website: http://geant4.cern.ch/support/userdocuments.shtml

[11] C. Suteau, M. Chiron and G. Arnaud. Improvement of MERCURE-6's general formalism for calculating gamma-ray buildup factors in multilayer shields. Nuc. Sci & Eng. 147, 43-55 (2004).

[12] F.L. Bronson. "Three new techniques for radiological characterisation and dose estimation". Presented at the international conference: Decommissioning challenges: An Industrial Reality. Sponsored by IAEA, ENS, OECD/NEA, SFEN November 23-25, 2003, Avignon, France

[13] H. Toubon, B. Nohl, S. Lefevre, M. Chiron, K. Boudergui, P. Pin. "New methodology for source location and activity determination in preparation of repairing or decommissioning activities". IRPA conference, 18 may 2006, Paris.

[14] A.G. Croff. ORIGEN2: A Versatile Computer Code for Calculating the Nuclide Compositions and Characteristics of Nuclear Materials. Nuclear Technology, 62, 335-352 (Sept. 1983)

[15] SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluations, ORNL/TM-2005/39, Version 5.1, Vols. I-III, Nov.2006.

[16] International Nuclear Verification Series No. 1 "Safeguards Techniques and equipment" 2003 Edition. International Atomic Energy Agency, Vienna.

[17] H. Toubon, A. Lebrun, L. Oriol, N Saurel, T. Gain and P. Pin. "Burn-up measurements coupling gamma spectrometry and neutron measurement". ENC2005 conference, VERSAILLES December 2005.

[18] M. Samson et al. "CESAR: a simplified evolution code applied to reprocessing application". RECOD 98, Nice (F) October 25-28, 1998

[19] J.M. Gomit, P. Cousinou, A. Duprey, C. Diop, J.P. Grouillier, L. Leyval, H. Toubon, E. Lejeune. "The new CRISTAL criticality safety package". Sixth International Conference on Nuclear Criticality Safety, Versailles, France, 20-24 September 1999 (ICNC'99).

[20] D.J. Whalen, D.A. Cardon, J.L. Uhle and J.S. Hendricks. "MCNP: Neutron Benchmark Problems", Los Alamos National Laboratory, LA-12212, 1993

[21] D.J. Whalen, D.E. Hollowell and J.S. Hendricks. "MCNP: Photon Benchmark Problems", Los Alamos National Laboratory, LA-12196, 1991.

[22] P. Baeten, M. Bruggeman, P. Chard, S. Croft, D. Parker, C. Zimmerman, M. Looman and S. Guardini. "Results of the ESARDA 'Reals' Prediction Benchmark Exercise"; ESARDA Bulletin No. 31, (April 2002).

[23] P. Chard et al. "Results of the ESARDA Monte Carlo 'Simple Case' Benchmark Exercise"; ESARDA Bulletin Nr 32, (March 2004).

[24] P. Peerani and M. Swinhoe. "Results of the ESARDA Multiplicity Benchmark Exercise"; ESARDA Bulletin No. 34.

[25] R. Venkataraman, F. Bronson, V. Atrashkevich, B.M. Young and M. Field. "Validation of in-Situ Object Counting System (ISOCS) mathematical efficiency calculation software", Proceedings of the 9th Symposium on Radiation Measurements Applications, Ann Arbor, MI, USA, May 11-14, 1998.

[26] R. Venkataraman, F. Bronson, V. Atrashkevich, B.M. Young and M. Field. "Validation of in-Situ Object Counting System (ISOCS) mathematical efficiency calculation software", Nucl. Inst and Methods in Phys Res A 422 (1999), pp 450 – 454.

[27] P. Peerani, G. Bosler, I. Cherradi and P. Schwalbach. "Computational Calibration of Neutron Collars for the Verification of HEU Fuel Elements", Proceeding of the 45th INMM Annual Meeting, Orlando (FL), 18-22 July 2004.

[28] P. Peerani. "Computational calibration of UNCL neutron collars for fresh fuel elements", JRC Technical Note, I.04.142, October 2004.

[29] P. Peerani and J. Tanaka. "Calibration of neutron collars for fresh fuel element verification", Proceeding of the 27th ESARDA Symposium on Safeguards and Nuclear Material Management, London (UK), 10-12 May 2005.

[30] P. Peerani. "Measurement of ^{235}U in fresh WWER fuel elements", Proceedings of the Tripartite Seminar, Obninsk (RF), 9-13 October 2006.

[31] H. Tagziria, P. Peerani, W. Koehne and P. Schwalbach. "On-Line Verification of MOX Fuel Magazines Using Monte Carlo Simulation", Proceeding of the 27th ESARDA Symposium on Safeguards and Nuclear Material Management, London (UK), 10-12 May 2005.

[32] H. Tagziria, P. Peerani, P. De Baere and P. Schwalbach. "Monte Carlo Modelling and Design Optimisation of a Neutron Coincidence Counter for the Verification of PuO_2 cans", Proceeding of the 10th International Symposium on Radiation Physics, Coimbra (PT), 17-22 September 2006.

[33] P. Peerani, M. Looman: "Computational modelling of NDA instruments for nuclear safeguards", Proc. 24th ESARDA Annual Meeting, Luxembourg, (June 2002), or "Monte Carlo simulation of neutron counters for safeguard applications", to be published on Nucl. Instr. & Meth. in Phys. Res. A.

[34] A.L Nichols, D.L Aldama and M. Verpelli. Handbook of Nuclear Data for Safeguards, INDC(NDC)-0502 (Jan. 2007).

[35] R.B. Firestone (Ed) Table of Isotopes (8th Edition), John Wiley & Sons, Inc (1996)

[36] LBNL Isotopes Project Nuclear Data Dissemination Home Page, http://ie.lbl.gov/toi.html

[37] M. Berger et al. XCOM: Photon Cross Section Database, NIST, Gaithersburg, MD, USA, http://physics.nist.gov/xcom

[38] J.F. Ziegler. SRIM/TRIM computer code for calculation of mass stopping powers of ions in matter. www.srim.org

[39] M.S. Zucker and N.E. Holden. "Parameters for several Plutonium Nuclides and ^{252}Cf of Safeguards Interest", Proc. 6th ESARDA Conf., Venice (I), 14-18 May 1984, 341.

[40] ENDF-6 Formats Manual. Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII. Document ENDF-102, Report BNL-NCS-44945-05.

[41] "Neutron reference radiations for calibrating neutron-measuring devices used for radiation protection purposes and for determining their response as a function of neutron energy", International Standard ISO8529:1989(E).

[42] P. Schillebeeckx, M. Looman and A Ravazzani. “Nuclear data required for non destructive assay of fissile and fertile material”, Presented at the seminar on fission, Point d’Oye, Belgium, Sept. 1999 (A useful paper describing the benefits for NDA safeguards measurements, of obtaining improved nuclear data)

[43] D. M. Cifarelli, W. Hage. “Models for a three parameter analysis of neutron signal correlation measurements for fissile material assay”, Nucl. Instr. and Meth. A251, (1986), 550-563.

[44] N. Ensslin et al. “Application Guide to Multiplicity Counting”, LA-13422-M, Los Alamos, (November 1998).

[45] S. Croft, R.D. McElroy and S.C. Kane. Coincidence gate utilisation factors for neutron correlation counters with up to three components in the die-away profile. Proceedings of the 11th International Conference on Environmental Remediation and Radioactive Waste Management, ICEM2007, September 2-6, 2007, Oud Sint-Jan Hospital Conference Center, Bruges, Belgium.

[46] I. Pazsit, A. Enqvist and L. Pal. A note on the multiplicity expressions in nuclear safeguards. Nucl. Inst and Methods in Phys Res A 603 (2009), pp 541 – 544.

[47] R. Gunnink. “MGA: A Gamma-Ray Spectrum Analysis Code for Determining Plutonium Isotopic Abundances, Vol. 1: Methods and Algorithms”, UCRL-LR-103220, Vol. 1 (1990).

[48] R. Gunnink, W.D. Ruther, P. Miller, J. Goerten, M. Swinhoe, H. Wagner, J. Verplancke, M. Bickel and S. Abousahl. “MGAU: A New Analysis Code for Measuring U-235 Enrichments in Arbitrary Samples”, UCRL-JC-114713, Lawrence Livermore National Laboratory, (1994).

[49] T.E. Sampson, G.W. Nelson, T.A. Kelly. “FRAM: A Versatile Code for Analyzing the Isotopic Composition of Plutonium from Gamma-Ray Pulse Height Spectra”, LA-11720-MS (1989).

[50] IGE: An Automatic software for the determination of actinides isotopics abundances. Proceedings of the International Workshop on Gamma Spectrometry Analysis codes for U and Pu isotopics, Oak Ridge, Tennessee, USA, Nov 03-07, 2008.

[51] E.E. Lewis and W.F. Miller Jr. “Computational methods of neutron transport”, Wiley-Interscience, New York, 1984.

[52] I. Lux and L. Koblinger. “Monte Carlo Particle Transport Methods: Neutron and Photon Calculations”, CRC Press, Boca Raton, 1991

[53] B. Morillon. “Une technique de biaisage automatique”, Proc. Advanced Monte Carlo computer programs for radiation transport. Saclay (France) 27th April 1993.

[54] T.E. Booth. “A Sample Problem for Variance Reduction in MCNP”, LANL Report LA-10363-MS (10/1985).

[55] H. Tagziria, P. Peerani, W. Koehne and P. Schwalbach. “Online verification of MOX Fuel Magazines in SMP with D4 detector”, Proceeding of the 27th ESARDA Symposium on Safeguards and Nuclear Material Management, London (UK), 10-12 May 2005.

[56] N. Roberts, H. Tagziria and D. Thomas. “Determination of the effective centres of the NPL neutron long counters”, NPL report DQL RN004, Nov. 2004.

[57] W.L. Oberkampf et al. “Estimation of Total Uncertainty in Modelling and Simulation”, Sandia Report, SAND2000-0824, April 2000

[58] W.L. Oberkampf et al. “Verification, Validation, and Predictive Capability in Computational Engineering and Physics”, SAND2003-3769, February 2003.

[59] United Kingdom Accreditation Service, The Expression of Uncertainty and Confidence in Measurement, UKAS Publication M 3003, Edition 1, 1997.

[60] [NASA] www.nianet.org/ecslectureseries/pdfs/isukapalli_030405.pdf (NASA/NIA ECS Lecture Series)

[61] PD 6461: Part 3: 1995: Vocabulary of Metrology, Part 3. Guide to the expression of uncertainty in measurement, International Organisation for Standardisation, Geneva.

[62] ASTM standard C1637 “Standard Terminology of C26.10 Nondestructive Assay Methods”. See www.astm.org/Standards/C1637.htm. Nuclear, Solar and Geothermal Energy. ASTM Book of Standards volume 12.01: Nuclear energy (I) Published by: ASTM International, 100 Barr Harbor Dr, PO Box C700, W. Conshohocken, PA 19428-2959. Revision Issued annually.

[63] ISO, International Organization for Standardization, Guide to the Expression of Uncertainty in Measurement, GUM, 1 Rue Varambé, Case Postale 56, CH 1221, Geneva, Switzerland.

[64] M. Grabe. Measurement Uncertainties in Science and Technology. Springer. ISBN 3-540-20944-7, 2005. http://www.springer.com/dal/home/generic/search/results?SGWID=1-40109-22-24419924-0, 2005.

[65] M. Grabe. "Principles of Metrological Statistics". Metrologia 23 (4): 213–19. doi:10.1088/0026-1394/23/4/006. http://www.iop.org/EJ/article/0026-1394/23/4/006/metv23i4p213.pdf, 1987.

[66] M. Grabe. "Estimation of Measurement Uncertainties—an Alternative to the ISO Guide". Metrologia 38 (2): 97–106. doi:10.1088/0026-1394/38/2/1. http://www.iop.org/EJ/article/0026-1394/38/2/1/me1201.pdf, 2001.

[67] The Alternative Error Model and its Impact on Traceability and Key Comparison, Joint BIPM-NPL Workshop on the Evaluation of Interlaboratory Comparison Data, NPL, Teddington, 19 September 2002.

[68] Draft ISO standard: “Determination of the characteristic limits (decision threshold, detection limit and limits of the confidence interval) for measurements of ionizing radiation – Fundamentals and application”, International Standard ISO/DIS-11929, draft 21/07/08.

Appendix A – Review of existing nuclear data and recommendations

In this appendix we provide a collection of neutron nuclear data. The references cited here are listed separately at the end of the Appendix, for clarity. The intention is not to be prescriptive in the sense that we do not intend absolutely to state that the user must necessarily follow our suggestions. We want simply to provide a support where a newcomer can find a complete and comprehensive set of nuclear data derived from experienced use of simulation tools and benchmark exercises. Of course anybody is totally free to use the nuclear data set that they trust provided that the fundamental principles drafted in these guidelines (and in particular in section 4.5 for nuclear data selection and validation) are met. Indeed, this principle would be good practice if, for example, adjusted data is available based on the results of a benchmark which is a close approximation to the problem.

A.1) Cross sections

All Monte Carlo codes for neutron transport simulation are provided with cross section libraries. For instance MCNP [1], one of the most frequently used codes, is distributed with its own set of libraries [2] and continuously new libraries are produced by different laboratories following the demand and the release of upgraded new evaluated nuclear data files (ENDF, JEFF, JENDL and others). A world-wide activity of validation of these data is permanently ongoing.

It is out of the scope of this paper to discuss and analyse the quality of MCNP libraries. Generally speaking, neutron counting requirements are not different from any other application of Monte Carlo codes and no specific improvements are needed, with maybe just the following exceptions.

A.2) Spontaneous fission data

The spontaneous fission rate is the primary quantity measured in passive neutron counting. In plutonium samples the most important contribution comes from the isotope ^{240}Pu, then contributions from the other even isotopes ^{242}Pu and ^{238}Pu follow, whereas the effect from odd isotopes is negligible. It is common practice to define a ^{240}Pu effective mass and to calibrate the counters with respect to this equivalent mass. Then the totalPu mass can be computed if the isotopic composition is known. The ^{240}Pu nuclear data are by far the most critical in most applications (with the exception of "heat-source" Pu where most of the Pu is ^{238}Pu).

The specific spontaneous fission neutron yield (number of neutrons produced per gram of isotope) is a fundamental datum because it appears directly in the conversion from fission rate to mass. This quantity is proportional to the product of the radioactive decay constant, the spontaneous fission branching ratio and the average number of emitted neutrons per fission event. It is surprising to see how there is not a clear agreement on such an important value even for the most important isotope.

For instance there is a difference of 1 to 2% between the most commonly accepted value in the Safeguard community [3 and 4] with respect to the most recent published data [5 and 6] (see Table I). Such a high uncertainty is not acceptable because it introduces directly an uncertainty of the same entity in the final result. Table II lists our suggested values for spontaneous fission decay data: with the exception of ^{240}Pu data, half-lives are taken from [4] and branching ratios from [6]. In Table III we report what we consider the best available multiplicity distributions, and the corresponding first three factorial moments. Note it is the factorial moments that are listed here.

Concerning the spectra of neutrons emitted by spontaneous fission, it is common practice to describe them in terms of predefined functions. The Maxwell distribution and the Watt distribution are the most popular functions for the description of energy distribution of fission neutrons. Table IV reports recommended values for the Watt distribution parameters for the main U and Pu isotopes [6].

Table V reports some different published data for 252Cf: the Watt spectrum from MCNP manual [1], the Maxwell spectrum recommended by ISO [10] and a recent work by Frohner [11] that is our preferred choice. The last two spectra are very similar and can be usually indifferently used without affecting significantly the results. On the contrary the spectrum produced using the MCNP Watt parameters is significantly harder and gives results less consistent with experimental measurements. The probability density function for the Watt spectrum is given by equation A1 where the constants a and b correspond to those listed in Table IV. The probability density function for the Maxwellian spectrum is given by equation A2 where the constants T corresponds to those listed in Table IV.

$$f(E) = C.\exp\left(-\frac{E}{a}\right)\sinh\left(bE\right)^{1/2} \quad \text{Eq A1}$$

$$f(E) = \frac{2}{\sqrt{\pi}.T^{3/2}} C.\sqrt{E}.e^{-E/T}.B \quad \text{Eq A2}$$

Reference	Half-life (y)	SF Branching ratio	SF Half-life (y)	Specific SF rate ($s^{-1}.g^{-1}$)
[3 and 4]	6560	5.65E-8	1.160E11	475
[5]	6568	5.70E-8	1.152E11	478
[6]		5.75E-8	1.141E11	485

Table I: Comparison among different published ^{240}Pu spontaneous fission data.

Isotope	SF Half-life (y)	Branching ratio	λSF (s^{-1})	Spontaneous fission rate ($.s^{-1}.g^{-1}$)
^{238}U	8.20E+15	5.45E-07	2.680E-24	6.776E-03
^{238}Pu	4.77E+10	1.84E-09	4.605E-19	1.165E+03
^{239}Pu	5.48E+15	4.40E-12	4.008E-24	1.010E-02
^{240}Pu	1.15E+11	5.70E-08	1.906E-19	4.791E+02
^{241}Pu	2.50E+15	5.74E-15	8.786E-24	2.195E-02
^{242}Pu	6.84E+10	5.50E-06	3.232E-19	7.989E+02
^{241}Am	1.05E+14	4.13E-12	2.092E-22	5.226E-01
^{252}Cf	85.6	3.092E-2	2.566E-10	6.130E+11

Table II: Suggested values for spontaneous fission decay data.

	^{238}U	^{238}Pu	^{240}Pu	^{242}Pu	^{252}Cf
References	[7]	[3, 9]	[8]	[8]	[8]
P(0)	0.0782	0.0541	0.0655	0.0683	0.0021
P(1)	0.2465	0.2054	0.2319	0.2302	0.0260
P(2)	0.3563	0.3802	0.3289	0.3343	0.1267
P(3)	0.2363	0.2248	0.2514	0.2469	0.2734
P(4)	0.0719	0.1079	0.1015	0.0991	0.3039
P(5)	0.0101	0.0276	0.0184	0.0181	0.1848
P(6)	0.0006	-	0.0024	0.0031	0.0657
P(7)	-	-	-	-	0.0154
P(8)	-	-	-	-	0.0020
νs_1	2.0097	2.2100	2.1563	2.1450	3.757
νs_2	1.6066	1.9783	1.9121	1.8971	5.983
νs_3	0.6369	0.9327	0.8894	0.8863	5.302

Table III: Multiplicity distributions for spontaneous fission.

Isotope	Watt spectrum parameters	
	a (MeV)	b (MeV^{-1})
^{238}U	0.6483	6.811
^{238}Pu	0.8478	4.169
^{240}Pu	0.7949	4.689
^{242}Pu	0.8192	4.367

Table IV: Suggested Watt parameters for spontaneous fission neutron spectra.

Reference	Distribution	a (MeV)	b (MeV^{-1})	T (MeV)
[1]	Watt	1.025	2.926	-
[10]	Maxwell	-	-	1.420
[11]	Watt	1.175	1.040	-

Table V: Comparison among different published data on ^{252}Cf.

In passive neutron coincidence counting (PNCC), where the measured quantity is the coincidence "Reals" count rate, no distinction is made between the different (even numbered) spontaneously fissioning isotopes. Measurement results are therefore normally expressed in terms of a ^{240}Pu effective mass, meff, where appropriate coefficients are defined to allow for the contribution from each of the even isotopes of Pu, to m_{eff}. The coefficients (see equation A3) depend on the nuclear data comprising of the spontaneous fission rate ($s^{-1}.g^{-1}$) and the second moment of the spontaneous fission neutron multiplicity distribution (that is, the parameter ν_{S2} with reference to equation 2 in section 4.5.2.1). These nuclear data are the subject of evaluation by experiment. A review paper [12] describes the evaluation of these parameters. Direct measurement of isotopically pure ^{238}Pu and ^{242}Pu standards is a powerful method of direct measurement of the m_{eff} coefficients. Such an exercise has been conducted [13, 14], which yielded coefficients of 2.71 and 1.66 (the values for A and B for ^{238}Pu and ^{242}Pu respectively. An important point here is the need to use a *consistent* set of coefficients, in order to achieve consistent results (for example for series of verification inspections). In terms of *absolute* nuclear data, however, it may still be worthwhile pursuing the determination, by measurement, of more accurate data.

$$m_{eff} = A.m(^{238}Pu) + m(^{238}Pu) + B.m(^{242}Pu) \quad \text{Eq A3}$$

A.3) Neutron-induced fission data

Beyond the cross sections, other nuclear data are required for a complete modelling of the induced fission reaction: the multiplicity distributions and the secondary neutron spectra. For the application of the point model it is enough to know just the average neutron yield and the factorial moments of the multiplicity distribution.

What makes things more difficult than in the case of spontaneous fission is that the above said quantities are not constant, but depend from the incident neutron energy. Complete multiplicity distributions for neutron induced fission (as a function of neutron energy up to 10 MeV) are available just for ^{235}U, ^{238}U and ^{239}Pu [15]. Table VI resumes the distributions just for E_n= 0 (thermal) and 1 MeV. As far as secondary neutron spectra are concerned, Table VII was derived from [1].

A.4) (alpha,n) reaction data

To compute the α factor appearing in the point model, we need to know the specific neutron yield from (α,n) reaction. This is the number of neutrons per second produced in a gram of a determined isotope. To produce a neutron the alpha particle from the decay of an actinide must interact with a light target nuclide (oxygen, fluorine, beryllium or others). Therefore the neutron yield is not simply a property of the alpha emitter, but also of the matrix of the material and sometimes it depends on the presence of impurities. In Table VIII we report the specific (α,n) neutron yields in uranium and plutonium oxides. Values available in literature [16, 17 and 4] are compared with those computed using the SOURCES-4A code [18].

For Monte Carlo modelling it is necessary to know also the spectrum of emitted neutrons. Differently from fission neutrons, there is not a simple parametric analytical expression for (α,n) neutron spectra. Neutron spectra from (α,n) reactions computed with SOURCES-4A for several plutonium isotopes in oxide matrix are listed in histogram form in Table IX. In the case of the AmLi source used for active neutron interrogation the theoretical spectrum computed by Geiger and van der Zwan [19] seem still to be a reasonably good model. The GvdZ spectrum is given in Table X. Experimentally measured spectra published more recently [20] could produce some improvements in the simulation. It is important to remark that the GvdZ spectrum is a theoretical spectrum of generated neutrons, its use is recommended when the detailed description of the source is available (material, composition, density, geometry); in this way all the modifications due to the neutron interactions with the source itself will be correctly taken into account. Experimentally measured spectra include already this information and are best suitable when the composition of the source is not known; moreover they can account for effects due to spurious reactions such as (α,n) on oxygen or impurities as beryllium. When using escaping neutron spectra it would be better not to model the source: leave the source location void and let neutrons be generated at the source surface.

References [21, 22 and 23] provide worthwhile additional reading, providing neutron spectral data from robust measurements of Am/Li and Am/F (α,n) neutron sources.

	^{235}U		^{238}U		^{239}Pu		^{241}Pu
Refer.	[15]		[15]		[15]		[3]
E_n	thermal	1 MeV	thermal	1 MeV	Thermal	1 MeV	thermal
P(0)	0.03172	0.02379	0.03965	0.02991	0.01088	0.00848	0.01015
P(1)	0.17171	0.15555	0.25295	0.20432	0.09949	0.07900	0.08857
P(2)	0.33620	0.32165	0.29395	0.29959	0.27489	0.25362	0.26490
P(3)	0.30397	0.31504	0.26445	0.29149	0.32692	0.32899	0.33454
P(4)	0.12695	0.14447	0.11118	0.13015	0.20461	0.23281	0.21325
P(5)	0.02668	0.03560	0.03123	0.03631	0.07268	0.08002	0.07607
P(6)	0.00263	0.00343	0.00593	0.00736	0.00973	0.01556	0.01200
P(7)	0.00014	0.00045	0.00054	0.00069	0.00063	0.00118	0.00052
P(8)	-	-	0.00012	0.00018	0.00017	0.00035	-
νi_1	2.4140	2.5237	2.2754	2.4306	2.8760	3.0089	2.9310
νi_2	2.3191	2.5507	2.1703	2.4480	3.3740	3.7054	3.4996
νi_3	1.1363	1.3335	1.1656	1.3566	2.0982	2.4321	2.2064

Table VI: Multiplicity distributions for neutron induced fission.

Nuclide	Spectrum function	Parameters	
		a (MeV)	B (MeV^{-1})
^{235}U	Watt	0.988	2.249
^{238}U	Watt	0.895	3.295
^{238}Pu	Maxwell	1.330	-
^{239}Pu	Watt	0.966	2.842
^{240}Pu	Maxwell	1.362	-
^{241}Pu	Maxwell	1.375	-
^{242}Pu	Maxwell	1.354	-
^{241}Am	Maxwell	1.330	-

Table VII: Parameters for induced fission neutron spectra.

	Published data on U/PuO_2		Computed with SOURCES-4A	
	Ref. [16, 4]	Ref. [17]	U/PuO_2	U_3O_8
^{234}U	3.0E+0	3.06E+0	3.03E+0	3.67E+0
^{235}U	7.1E-4	7.18E-4	7.19E-4	-
^{236}U	2.4E-2	2.41E-2	2.39E-2	-
^{238}U	8.3E-5	8.22E-5	8.36E-5	1.01E-4
^{238}Pu	1.34E+4	1.38E+4	1.386E+4	-
^{239}Pu	3.81E+1	3.97E+1	3.940E+1	-
^{240}Pu	1.41E+2	1.46E+2	1.455E+2	-
^{241}Pu	1.3E+0	1.34E+0	1.333E+0	-
^{242}Pu	2.0E+0	2.12E+0	2.112E+0	-
^{241}Am	2.69E+3	2.75E+3	2.767E+3	-

Table VIII: (α,n) neutron yields in uranium and plutonium oxides.

Energy boundaries (MeV)	5.00	4.95	4.90	4.85	4.80	4.75	4.70	4.65
	4.60	4.55	4.50	4.45	4.40	4.35	4.30	4.25
	4.20	4.15	4.10	4.05	4.00	3.95	3.90	3.85
	3.80	3.75	3.70	3.65	3.60	3.55	3.50	3.45
	3.40	3.35	3.30	3.25	3.20	3.15	3.10	3.05
	3.00	2.95	2.90	2.85	2.80	2.75	2.70	2.65
	2.60	2.55	2.50	2.45	2.40	2.35	2.30	2.25
	2.20	2.15	2.10	2.05	2.00	1.95	1.90	1.85
	1.80	1.75	1.70	1.65	1.60	1.55	1.50	1.45
	1.40	1.35	1.30	1.25	1.20	1.15	1.10	1.05
	1.00	0.95	0.90	0.85	0.80	0.75	0.70	0.65
	0.60	0.55	0.50	0.45	0.40	0.35	0.30	0.25
	0.20	0.15	0.10	0.05	0.00			
^{238}Pu	1.69E-04	1.79E-04	1.85E-04	1.92E-04	1.99E-04	2.07E-04	2.16E-04	2.25E-04
	2.37E-04	2.51E-04	3.30E-04	6.13E-04	9.54E-04	1.30E-03	1.65E-03	2.00E-03
	2.36E-03	2.73E-03	3.27E-03	3.84E-03	4.55E-03	5.33E-03	6.11E-03	6.77E-03
	7.43E-03	8.16E-03	8.84E-03	9.57E-03	1.05E-02	1.11E-02	1.18E-02	1.26E-02
	1.34E-02	1.43E-02	1.53E-02	1.62E-02	1.69E-02	1.76E-02	1.82E-02	1.90E-02
	1.98E-02	2.09E-02	2.19E-02	2.23E-02	2.25E-02	2.26E-02	2.27E-02	2.30E-02
	2.35E-02	2.36E-02	2.33E-02	2.31E-02	2.28E-02	2.23E-02	2.20E-02	2.17E-02
	2.08E-02	1.98E-02	1.89E-02	1.83E-02	1.75E-02	1.70E-02	1.62E-02	1.51E-02
	1.39E-02	1.32E-02	1.26E-02	1.20E-02	1.14E-02	1.07E-02	9.90E-03	9.42E-03
	8.65E-03	8.02E-03	7.80E-03	7.28E-03	6.83E-03	6.49E-03	6.19E-03	6.07E-03
	5.80E-03	5.49E-03	5.42E-03	5.29E-03	5.31E-03	5.14E-03	5.02E-03	5.05E-03
	5.12E-03	5.04E-03	4.96E-03	4.77E-03	4.34E-03	4.18E-03	4.18E-03	4.17E-03
	4.18E-03	3.74E-03	2.96E-03	1.85E-03				
^{239}Pu	1.23E-04	1.35E-04	1.44E-04	1.52E-04	1.60E-04	1.71E-04	1.83E-04	1.94E-04
	2.09E-04	2.28E-04	2.45E-04	2.70E-04	2.89E-04	3.03E-04	3.17E-04	3.37E-04
	3.64E-04	6.39E-04	1.03E-03	1.24E-03	1.61E-03	2.04E-03	2.48E-03	2.79E-03
	3.21E-03	4.07E-03	4.96E-03	5.90E-03	7.02E-03	7.85E-03	8.72E-03	9.77E-03
	1.08E-02	1.19E-02	1.33E-02	1.44E-02	1.53E-02	1.61E-02	1.69E-02	1.79E-02
	1.90E-02	2.04E-02	2.16E-02	2.25E-02	2.34E-02	2.42E-02	2.50E-02	2.57E-02
	2.62E-02	2.66E-02	2.68E-02	2.70E-02	2.72E-02	2.68E-02	2.63E-02	2.59E-02
	2.48E-02	2.34E-02	2.23E-02	2.15E-02	2.05E-02	1.99E-02	1.88E-02	1.75E-02
	1.60E-02	1.50E-02	1.43E-02	1.35E-02	1.28E-02	1.18E-02	1.08E-02	1.02E-02
	9.26E-03	8.61E-03	8.48E-03	7.94E-03	7.27E-03	6.49E-03	5.82E-03	5.57E-03
	5.16E-03	4.71E-03	4.56E-03	4.35E-03	4.37E-03	4.14E-03	4.00E-03	4.03E-03
	4.25E-03	4.61E-03	5.02E-03	5.32E-03	5.18E-03	5.06E-03	5.06E-03	4.99E-03
	4.86E-03	4.20E-03	3.15E-03	1.81E-03				
^{240}Pu	1.26E-04	1.37E-04	1.46E-04	1.54E-04	1.63E-04	1.73E-04	1.85E-04	1.96E-04
	2.11E-04	2.29E-04	2.47E-04	2.71E-04	2.90E-04	3.04E-04	3.19E-04	3.37E-04
	3.91E-04	7.04E-04	1.10E-03	1.31E-03	1.67E-03	2.10E-03	2.54E-03	2.85E-03
	3.33E-03	4.21E-03	5.09E-03	6.02E-03	7.14E-03	7.97E-03	8.83E-03	9.87E-03
	1.09E-02	1.20E-02	1.33E-02	1.44E-02	1.54E-02	1.61E-02	1.70E-02	1.79E-02
	1.90E-02	2.04E-02	2.16E-02	2.25E-02	2.34E-02	2.42E-02	2.50E-02	2.57E-02
	2.62E-02	2.66E-02	2.67E-02	2.69E-02	2.71E-02	2.66E-02	2.61E-02	2.57E-02
	2.46E-02	2.33E-02	2.22E-02	2.14E-02	2.04E-02	1.98E-02	1.87E-02	1.74E-02
	1.59E-02	1.50E-02	1.42E-02	1.35E-02	1.27E-02	1.18E-02	1.08E-02	1.02E-02
	9.24E-03	8.59E-03	8.46E-03	7.92E-03	7.22E-03	6.44E-03	5.83E-03	5.58E-03
	5.18E-03	4.73E-03	4.59E-03	4.39E-03	4.41E-03	4.18E-03	4.04E-03	4.07E-03
	4.29E-03	4.64E-03	5.06E-03	5.35E-03	5.17E-03	5.04E-03	5.04E-03	4.96E-03
	4.83E-03	4.17E-03	3.13E-03	1.80E-03				

^{241}Pu	7.37E-05	8.77E-05	9.76E-05	1.07E-04	1.18E-04	1.30E-04	1.44E-04	1.57E-04
	1.75E-04	1.97E-04	2.17E-04	2.46E-04	2.69E-04	2.85E-04	3.03E-04	3.25E-04
	3.49E-04	3.74E-04	3.95E-04	4.19E-04	4.44E-04	4.91E-04	8.47E-04	1.20E-03
	1.56E-03	2.02E-03	2.68E-03	3.41E-03	4.15E-03	4.76E-03	5.73E-03	6.97E-03
	8.19E-03	9.51E-03	1.11E-02	1.24E-02	1.35E-02	1.44E-02	1.54E-02	1.65E-02
	1.78E-02	1.94E-02	2.09E-02	2.20E-02	2.30E-02	2.39E-02	2.49E-02	2.61E-02
	2.72E-02	2.82E-02	2.89E-02	2.92E-02	2.95E-02	2.94E-02	2.94E-02	2.94E-02
	2.85E-02	2.70E-02	2.55E-02	2.43E-02	2.31E-02	2.23E-02	2.11E-02	1.95E-02
	1.77E-02	1.66E-02	1.57E-02	1.48E-02	1.40E-02	1.28E-02	1.17E-02	1.09E-02
	9.81E-03	9.05E-03	8.89E-03	8.26E-03	7.67E-03	7.05E-03	6.50E-03	6.14E-03
	5.45E-03	4.73E-03	4.23E-03	3.63E-03	3.51E-03	3.19E-03	2.96E-03	2.93E-03
	3.16E-03	3.56E-03	4.05E-03	4.40E-03	4.48E-03	4.79E-03	5.34E-03	5.60E-03
	5.56E-03	4.91E-03	3.71E-03	2.13E-03				
^{242}Pu	7.29E-05	8.70E-05	9.69E-05	1.07E-04	1.17E-04	1.29E-04	1.44E-04	1.57E-04
	1.74E-04	1.96E-04	2.17E-04	2.46E-04	2.69E-04	2.85E-04	3.02E-04	3.25E-04
	3.48E-04	3.74E-04	3.95E-04	4.18E-04	4.33E-04	4.73E-04	8.16E-04	1.17E-03
	1.54E-03	1.99E-03	2.65E-03	3.38E-03	4.10E-03	4.71E-03	5.67E-03	6.92E-03
	8.14E-03	9.47E-03	1.10E-02	1.23E-02	1.34E-02	1.44E-02	1.53E-02	1.65E-02
	1.78E-02	1.94E-02	2.09E-02	2.20E-02	2.30E-02	2.39E-02	2.49E-02	2.61E-02
	2.72E-02	2.82E-02	2.89E-02	2.93E-02	2.95E-02	2.94E-02	2.94E-02	2.94E-02
	2.86E-02	2.71E-02	2.56E-02	2.44E-02	2.31E-02	2.24E-02	2.11E-02	1.95E-02
	1.77E-02	1.66E-02	1.57E-02	1.48E-02	1.40E-02	1.28E-02	1.17E-02	1.09E-02
	9.82E-03	9.05E-03	8.90E-03	8.26E-03	7.68E-03	7.06E-03	6.51E-03	6.15E-03
	5.46E-03	4.74E-03	4.23E-03	3.63E-03	3.49E-03	3.17E-03	2.94E-03	2.91E-03
	3.14E-03	3.54E-03	4.03E-03	4.38E-03	4.47E-03	4.78E-03	5.33E-03	5.61E-03
	5.57E-03	4.92E-03	3.72E-03	2.14E-03				
^{241}Am	1.69E-04	1.78E-04	1.85E-04	1.91E-04	1.98E-04	2.06E-04	2.16E-04	2.25E-04
	2.36E-04	2.51E-04	3.01E-04	5.73E-04	9.11E-04	1.26E-03	1.61E-03	1.97E-03
	2.32E-03	2.68E-03	3.18E-03	3.75E-03	4.47E-03	5.25E-03	6.03E-03	6.70E-03
	7.36E-03	8.09E-03	8.77E-03	9.51E-03	1.04E-02	1.11E-02	1.17E-02	1.26E-02
	1.34E-02	1.43E-02	1.53E-02	1.62E-02	1.69E-02	1.75E-02	1.82E-02	1.90E-02
	1.98E-02	2.09E-02	2.19E-02	2.23E-02	2.25E-02	2.26E-02	2.28E-02	2.30E-02
	2.35E-02	2.37E-02	2.34E-02	2.32E-02	2.29E-02	2.24E-02	2.21E-02	2.18E-02
	2.09E-02	1.98E-02	1.90E-02	1.84E-02	1.76E-02	1.70E-02	1.62E-02	1.52E-02
	1.40E-02	1.32E-02	1.26E-02	1.20E-02	1.15E-02	1.07E-02	9.92E-03	9.42E-03
	8.67E-03	8.03E-03	7.81E-03	7.29E-03	6.83E-03	6.48E-03	6.19E-03	6.06E-03
	5.79E-03	5.48E-03	5.41E-03	5.28E-03	5.30E-03	5.12E-03	5.01E-03	5.03E-03
	5.13E-03	5.06E-03	4.98E-03	4.79E-03	4.36E-03	4.18E-03	4.18E-03	4.17E-03
	4.17E-03	3.73E-03	2.95E-03	1.84E-03				

Table IX: SOURCES-4A Neutron spectra for (alpha,n) reactions from plutonium isotopes present in PuO_2 [18].

Energy boundaries (MeV)	1.0E-11	0.001	0.002	0.003	0.004	0.005	0.006
	0.007	0.008	0.009	0.01	0.02	0.03	0.04
	0.05	0.06	0.07	0.08	0.09	0.1	0.11
	0.12	0.13	0.14	0.15	0.16	0.17	0.18
	0.19	0.2	0.22	0.24	0.26	0.28	0.3
	0.32	0.34	0.36	0.38	0.4	0.42	0.44
	0.46	0.48	0.5	0.52	0.54	0.56	0.58
	0.6	0.62	0.64	0.66	0.68	0.7	0.72
	0.74	0.76	0.78	0.8	0.82	0.84	0.86
	0.88	0.9	0.92	0.94	0.96	0.98	1
	1.02	1.04	1.06	1.08	1.1	1.12	1.14
	1.16	1.18	1.2	1.22	1.24	1.26	1.28
	1.3	1.32	1.34	1.36	1.38	1.4	1.44
	1.48	1.5	1.52	1.54			
Spectrum in histogram form (MeV^{-1})	0	0.00004	0.00007	0.00009	0.00011	0.00013	0.00014
	0.00015	0.00017	0.00018	0.00019	0.00247	0.00352	0.00460
	0.00585	0.00723	0.00852	0.00966	0.01055	0.01130	0.01187
	0.01242	0.01292	0.01332	0.01343	0.01333	0.01322	0.01311
	0.01297	0.01284	0.02542	0.02493	0.02448	0.02404	0.02355
	0.02308	0.02261	0.02215	0.02173	0.02119	0.02071	0.02034
	0.01978	0.01935	0.01894	0.01844	0.01803	0.01758	0.01715
	0.01676	0.01626	0.01590	0.01552	0.01511	0.01471	0.01435
	0.01401	0.01363	0.01329	0.01294	0.01263	0.01230	0.01201
	0.01171	0.01141	0.01110	0.01082	0.01051	0.01022	0.00995
	0.00963	0.00933	0.00902	0.00868	0.00835	0.00796	0.00759
	0.00718	0.00677	0.00632	0.00591	0.00550	0.00509	0.00467
	0.00428	0.00387	0.00346	0.00305	0.00267	0.00228	0.00332
	0.00174	0.00032	0.00003	0.00000			

Table X: Geiger and van der Zwan spectrum of the AmLi neutron source [19].

References for Appendix A

[1] J.F. Briesmeister. "MCNP – A General Monte Carlo N-Particle Transport Code", LA-13709-M, Los Alamos (March 2000).

[2] RSICC Data Library Collection. "MCNPDATA: Standard Neutron, Photon and Electron Data Libraries for MCNP4C", DLC-200, Oak Ridge (March 2001).

[3] M.S. Zucker and N.E. Holden. "Parameters for several Plutonium Nuclides and ^{252}Cf of Safeguards Interest", Proc. 6th ESARDA Conf., Venice (I), 14-18 May 1984, 341.

[4] D. Reilly, N. Ensslin, H. Smith Jr. and S. Kreiner. "Passive Nondestructive Assay of Nuclear Materials", NUREG/CR-5550, LA-UR-90-732, (March 1991).

[5] JEFF2.2 Evaluated Nuclear Data File, (July 1993).

[6] E.F. Shores. "Data Updates for the SOURCES-4A Computer Code", LA-UR-00-5016, Los Alamos, (October 2000).

[7] M.R. Looman, P. Peerani and P. Schillebeeckx. "An Overview of NDA Instruments modelled with the MCNP-PTA Code at JRC Ispra", Proc. 23rd ESARDA Conf., Bruges (B), 8-10 May 2001.

[8] J.W. Boldeman and M.G. Hines. "Prompt Neutron Emission Probabilities following Spontaneous and Thermal Neutron Fission", Nuclear Science Engineering, 91, (1985), 114.

[9] D.A. Hicks, J. Ise and R.V. Pyle. "Probabilities of Prompt-Neutron Emission from Spontaneous Fission", Physical Review 101, (1956), 1016.

[10] "Neutron reference radiations for calibrating neutron-measuring devices used for radiation protection purposes and for determining their response as a function of neutron energy", International Standard ISO8529:1989(E).

[11] F.H. Frohner. "Evaluation of ^{252}Cf Prompt Fission Neutron Data from 0 to 20 MeV by Watt spectrum fit", Nuclear Science Engineering, 106, (1990), 345-352.

[12] P.M.J. Chard and S. Croft. "A database of ^{240}Pueffective and ^{235}Ueffective coefficients for various fertile and fissile isotopes". Proceedings of the 19th ESARDA Symposium on Safeguards & Nuclear Material Management, Montpellier, France, 13-15 May 1997.

[13] H. Ottmar, P. van Belle, S. Croft, P.M.J. Chard, L. C-A. Bourva and U. Blohm-Hieber. "An Empirical Measurement of the Specific 240Pu-Effective Mass of 238Pu and 242Pu". Proceedings of the 21st ESARDA Symposium on Safeguards & Nuclear Material Management, Sevilla, Spain, 4-6 May 1999.

[14] S. Croft, L.C-A Bourva, D.R. Weaver and H. Ottmar. "240Pu Effective Mass of 238Pu and 242Pu in Relation to Passive Neutron Coincidence and Multiplicity Counting". Journal of Nuclear Materials Management. Volume 30 (1), 2001.

[15] M. S. Zucker and N. E. Holden. "Neutron Multiplicity for Neutron Induced Fission of ^{235}U, ^{238}U and ^{239}Pu as a Function of Neutron Energy", IAEA-SM-293/122, Vienna (1986), 329.

[16] R.T. Perry and B.W. Wilson. "Neutron Production from (α,n) Reactions and Spontaneous Fission in ThO_2, UO_2 and (U,Pu) O_2 Fuels", LA-8869-MS, Los Alamos, (June 1981).

[17] S. Croft. "The calculation of the Enhancement of the (α,n) Production Rate in PuO_2 and MOX powders caused by the Presence of Moisture", Proc. 17th ESARDA Conf., Aachen (D), 9-11 May 1995, 419.

[18] W.B. Wilson et al. "SOURCES-4A: a Code for calculating (α,n), Spontaneous Fission and Delayed Neutron Sources and Spectra", LA-13639-MS, Los Alamos, (September 1999).

[19] K.W. Geiger and L. van der Zwan. "The Neutron Spectra and the resulting Fluence-kerma Conversions for ^{241}Am-Li(α,n) and 210Po-Li(α,n) Sources", Health Physics, 21 (1971) 120-123.

[20] H. Tagziria, N.J. Roberts and D.J. Thomas. "Measurement of the ^{241}Am–Li radionuclide neutron source spectrum", Nuclear Instruments and Methods in Physics Research Section A, Vol. 510, Issue 3, (September 2003), 346-356.

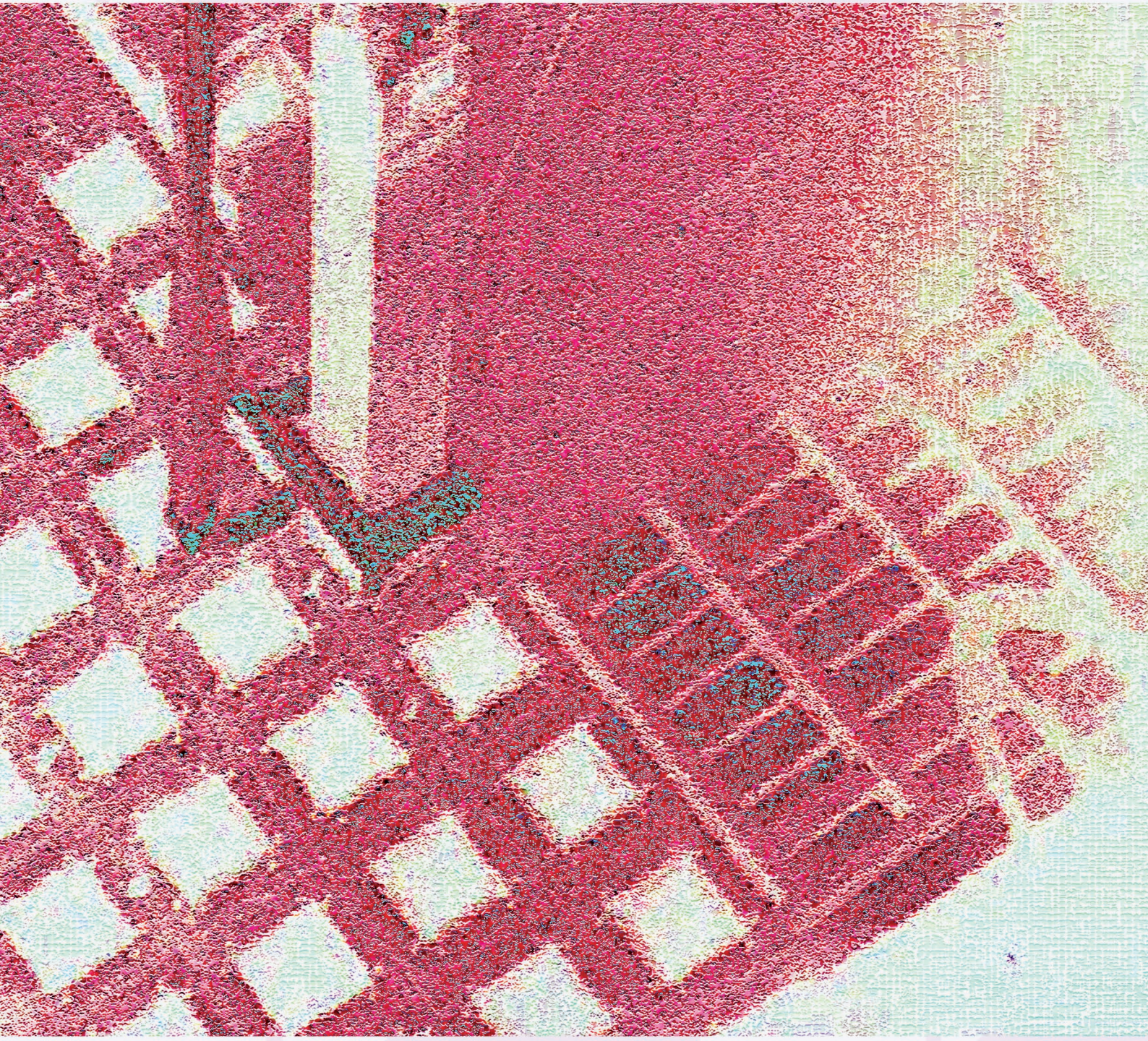
[21] J.G. Owen, D.R. Weaver and J. Walker. "The calibration of a 3He spectrometer and its use to measure the spectrum of neutrons from an Am/Li source". Nuclear Instrumentation and Methods. 188 (1981), 579-593.

[22] D.R. Weaver, J.G. Owen and J. Walker. "The neutron spectrum from a 5Ci Am/Li neutron source". Nuclear Instrumentation and Methods. 198 (1982), 599-602

[23] J.G. Owen, D.R. Weaver and J. Walker. "Neutron spectra from Am/F and Am/Li (α,n) sources". International conference on Nuclear Data for Science and Technology, Antwerp, 6-10 Sept (1982), 492-495.

The cover of this Issue is inspired by its title ‘Non-Destructive Analysis’.
It shows an image that seems to have a second layer on top, or looks like a mirror, but in fact it is not.
It means ‘modifying a picture without destroying it’, an artistic translation of the Bulletin’s title.

LB-AB-09-042-EN-C



Publications Office

www.jrc.ec.europa.eu/esarda