ESARDA NDA WORKING GROUP

RESULTS OF THE MONTE CARLO "SIMPLE CASE" BENCHMARK EXERCISE

November 2003

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1 INTRODUCTION

The ESARDA Non-Destructive Assay (NDA) Working Group (WG) has previously organised several intercomparison exercises, aimed at establishing the performance of NDA techniques currently employed in safeguards. These include round - robin exercises where laboratories make comparative NDA measurements on a set of samples, and intercomparisons for data analysis codes.

Passive and Active Neutron Coincidence Counting is widely used in safeguards for the verification of fuel pins and assemblies, the measurement of the fissile content of scrap residues from reprocessing activities, and the assay of individual fuel pellets for process control.

The use of Monte Carlo modelling is becoming increasingly widespread as a tool for reducing the reliance upon experiment (which often requires the use of costly standards) for calibration of neutron coincidence counting systems. Increasing availability of powerful computers means that the complexity with which physical systems can be modelled is increasing. However, the accuracy of the results obtained is also influenced by the nuclear data constants which are used by the program, as well as the interpretational models used to convert calculated quantities into measurement parameters. In this context, there is increasing interest in the safeguards community in establishing nuclear data sets and methodologies which can be used reliably for these applications.

The NDA WG recently published [1], the results of an Intercomparison Exercise, the "Reals benchmark exercise", in which a number of participants used MCNP™, an established Monte Carlo code in safeguards, to predict the coincidence counting rates for a standard Euratom Active Neutron Coincidence Collar. The emphasis of this exercise was placed on studying the methods used when applying MCNP™, that is, the interpretational models which are used to convert the raw calculated quantities, into quantities which are relevant to measurement, namely counting rates. To this end, participants used the same nuclear data for the actual MCNP™ runs, with a fixed, predefined geometry model, but different interpretational models. The results of comparisons with experiment demonstrated that predictions could generally be made to an accuracy of 5 - 10 %. However, due to uncertainties in the accuracy of the nuclear data constants used (neutron cross-sections, neutron source spectra, thermal neutron scattering treatments), it is not clear whether, nor by how much, it is possible to further improve on this figure, nor what are the factors which determine the fundamental limits. Furthermore, the relative contributions to the differences in results from i) differences in the nuclear data used in the interpretational models, and ii) differences in the physics of the interpretational models themselves, were not clear. Although the MCNP™ modelling was based on as accurate a geometry model as possible, certain physical effects were not taken into account, such as the true effective active length of the detectors, and the fractional wall effect losses. This means that there is an additional, as yet unquantified, source of uncertainty which undoubtedly affects the level of agreement which can generally be expected between experiment and calculation.

A new "Simple Case" benchmark Intercomparison Exercise was launched, intended to study the importance of the fundamental nuclear data constants, physics treatments and geometry model approximations, employed by Monte Carlo codes in common use. The exercise was also directed at determining the level of agreement which can be expected between measured and calculated quantities, using current state of the art modelling codes and techniques. To this end, measurements and Monte Carlo calculations of the Totals (or Gross) neutron count rates have been performed using a simple moderated ^{3}He filled cylindrical proportional counter array or "slab monitor" counting geometry. It was decided to select a very simple geometry for this exercise. This was to ensure that there is little opportunity to introduce uncertainties into the results as a consequence of errors in the geometry modelling due to the geometry being not well defined. Furthermore the use of a standard, well characterised detector system minimises the risk of introducing additional uncertainties due to errors in modelling details such as moderator density, detector fill pressures, etc. so that there is minimum potential for uncertainty due to unquantifiable variables in the geometry. The comparison between measurement and calculation was directed at the simplest possible measurable quantity, namely the Totals counting rate, in order to direct the analysis towards the influence of nuclear data, physics treatment and geometry approximations, rather than the details of a potentially complex interpretational model (the Reals Prediction benchmark focussed on this).

It was agreed that Monte Carlo modelling would be carried out by participants from as wide a range of organisations as possible. By requesting that the participants each use their preferred codes, the exercise facilitated a comparison of all the codes in common use for NDA applications in safeguards. Furthermore, the intention was for each participating group to develop their own independent geometry model, based on detailed drawings of the as – built detector system, supplied by the project co-ordinator as obtained from the manufacturers of the equipment. This gives a good overall understanding of the range of possible geometry modelling approximations and their effects. The simple geometry treated in this exercise, gives a high degree of control over the geometry variables. It was anticipated that each group would use their own preferred nuclear data sets and physics treatments, such that at the end of the exercise, analysis would allow sensitivity studies to be performed for the various factors.

By benchmarking against the experiments, it was hoped that a consensus could be reached for a preferred set of data to be used for neutron assay systems as well as providing insight into the fundamental accuracy limitations of the Monte Carlo modelling.

This report describes the scope of the measurements and calculations, and gives a summary of the results obtained (the results were presented earlier [2]). The results are compared, and sensitivity studies shown, to determine the influence of the various parameters. It is considered that this new "Simple Case Benchmark" intercomparison exercise can potentially offer interesting and useful results to the safeguards community. The results will benefit both the NDA specialist interested in the accuracy with which Monte Carlo modelling can be used for design / calibration work and the inspector, who needs to keep up to date with the expected performance of NDA instruments and predictive tools which are increasingly being used to assist calibrations of NDA equipment.

2 PROJECT ORGANISATION

The project co-ordinator, Dr P.M.J.Chard of the United Kingdom Atomic Energy Authority (UKAEA), Dounreay, initially specified a simple slab geometry configuration, including various thicknesses of moderator and shielding, in conjunction with an array of ^{3}He proportional counters and a ^{252}Cf spontaneous fission neutron source. This slab monitor geometry comprised a standard “N50” neutron slab counter, as commonly used by EURATOM for monitoring Pu holdup and general monitoring of neutron radiation levels. The experiments were conducted independently of the modelling, at Harwell Laboratory, Oxfordshire, in the United Kingdom. None of the participants performing Monte Carlo modelling were given any details of the measurements, so as to ensure that the modelling was performed “blind”. Likewise, the experimenters were given no information on the modelling results, prior to completion of the measurements and assembly of the full set of the results for checking and analysis by the project co-ordinator.

A specification document was issued in order to fully describe the experimental set-up, in sufficient detail that an accurate Monte Carlo geometry model could be setup by each participant, and also to give some guidance as to the range of measurements and calculations to be performed. The various geometry configurations to be studied (additional moderator and absorber slabs) were defined in detail. This specification document was distributed for comment and finally issued for participants to commence their modelling. Following feedback from a number of the participants, clarification was given via emails to all the participants, which was subsequently incorporated into a revised version [3] of the specification document.

The specification document also gave some indications as to what nuclear data and physics treatments would be appropriate for this study. However, participants were encouraged to identify their own preferred data sets, and also to use their knowledge of alternative data sets to perform sensitivity studies in the Monte Carlo runs.

Following advertisement of the exercise, interest was expressed from various organisations, with the intention of using the most commonly used codes. In total, 10 groups participated in the modelling phase of the exercise; 7 used MCNP^{TM} while 2 used MCBEND while 1 used TRIPOLI. These participants to the exercise are summarised in Table 1. MCNP^{TM} is a modern standard code for this type of radiation transport modelling in support of the design and calibration of NDA systems for nuclear material safeguards applications. MCBEND was designed as a shielding code and, as such, has not been widely applied to NDA problems. Similarly, TRIPOLI is not widely used for safeguards / NDA applications. However, it is believed that these codes have the functionality required to perform this type of modelling.

	Group	Role
A	BNFL Instruments	MCNP 4C
B	CEA Saclay	TRIPOLI 4.3
C	CEA Cadarache	MCNP 4C2
D	RMTC IPPE	MCNP 4B
E	BNFL	MCBEND 9E (RU0)
F	NRA Argentina	MCNP 4B
G	CEN IPSN	MCNP 4B
H	Serco Assurance	MCBEND 9E (RU2)
I	IPP Obninsk	MCNP 4B
J	JRC Ispra	MCNP 4B
	Canberra - Harwell	Experiments and data analysis
	UKAEA	Project co-ordination

Table 1. Summary of participants and their roles

3 SLAB MONITOR AND DETECTOR GEOMETRY

The model N50 neutron slab monitor [4], originally designed with the aid of benchmarked MCNP^{TM} modelling, consists of four ^{3}He detectors embedded in a polyethylene moderator. The exact details of the geometry including the detector active lengths, fill pressure, wall thickness and materials, and also the geometry and materials of the moderator and its stainless steel casing, are given in the technical specification document [3]. Details are also given on such details as the detector dead spaces, and the dimensions of the holes into which they are embedded, so that such details could be included in the participant's Monte Carlo models. A summary of the basic N50 geometry is shown in Figure 1.

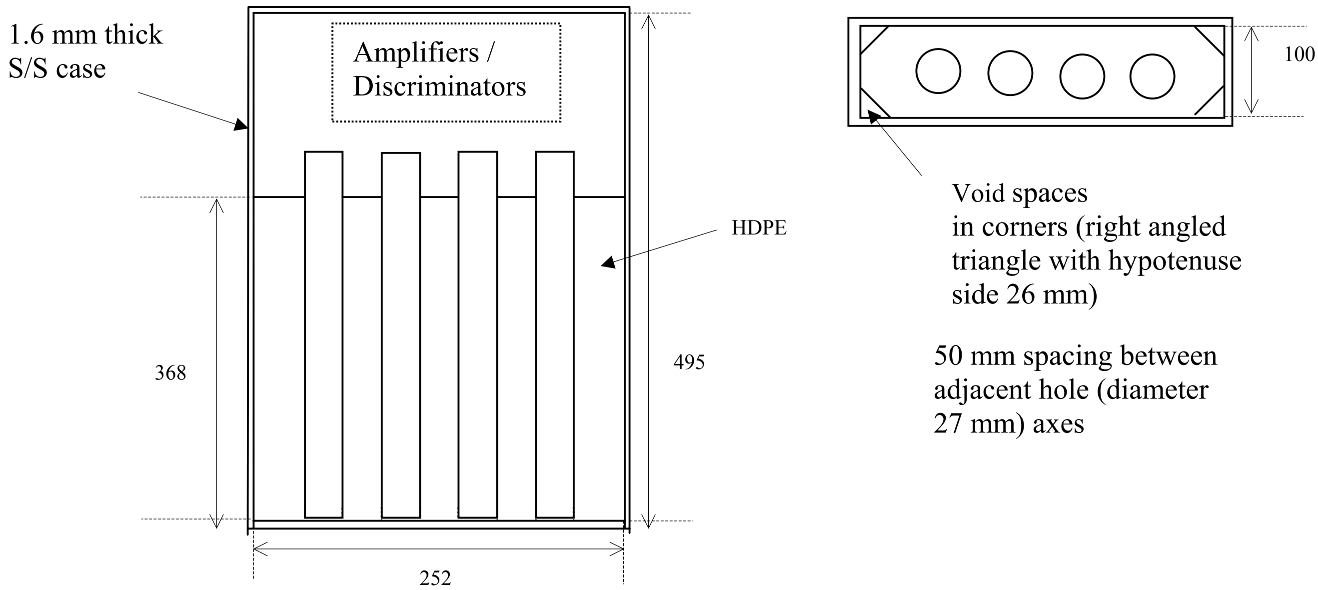


Figure 1. N50 configuration. Dimensions are given in mm. S/S indicates stainless steel. HDPE indicates High Density Polyethylene.

3.1 Model simplifications and assumptions

The following assumptions were made by the participants, based on measured values. Full details of these can be found in the technical specification document [3].

- Polyethylene density best estimate of 0.94 g.cm^{-3}, based on information from the HDPE supplier. Note: Supplier's information indicated a possible range of densities from 0.90 – 0.97 g.cm^{-3}. The selected value is supported by a measured value of (0.95 ± 0.01) for the N50 moderator based on weight and dimension measurements allowing for "cut away" regions in the geometry.
- Detector walls Stainless Steel 7.93 g.cm^{-3}, type 347 (18 wt. % Cr, 9 wt. % Ni and 0.08 wt. % C)
- Slab casing Stainless Steel 7.93 g.cm^{-3}, type 304 (18 wt. % Cr, 10 wt. % Ni and 0.03 wt. % C)
- Cadmium metal with a density of 8.65 g.cm^{-3} and natural isotopic abundance.
- Detectors filled at 20 degrees Celcius with 4 atm. ^{3}He, equating to a fill density of 0.00050172 g.cm^{-3} (as calculated using the ideal gas law).
- ^{252}Cf source should be considered as a cylinder with outer height 10 mm, outer diameter 7.8 mm, and wall (S/S grade 347, density 7.93 g.cm^{-3}) thickness 1.6 mm. The author's direct experience shows the effect of this encapsulation on the detection efficiency is negligible (< 0.1 %), and so there is no concern over the accuracy of this part of the modelling.
- Model the system within an arbitrary 5 m radius air – filled sphere, centred at the point half way between the source and the N50 front face (on a perpendicular line). This allows for air scatter.
- Assume that the system is neutronically isolated from the environment (most importantly the concrete floor and walls), i.e that the effects of floor / wall scatter are negligible and that they need not be included in the model. In practice the experiment was setup at the centre of a room at a large distance from the walls, and also a cadmium sheet was placed on the ground. Measurements showed that this assumption is approximately valid, and a bounding case study was performed to

place an upper estimate on its effect. Experimentally this involved performing measurements as a function of source – detector separation.

- According to [5], the density of air at sea level is 0.001225 $g.cm^{-3}$. The composition (by volume %) of N_2 : O_2 : Ar : CO_2 : Ne : He : CH_4 : Kr : H_2 : N_2O : Xe : Rn is given as 78.09 : 20.95 : 0.93 : 0.03 : 1.8×10^{-3} : 5.2×10^{-4} : 2.0×10^{-4} : 1.0×10^{-4} : 5.0×10^{-5} : 5.0×10^{-5} : 9.0×10^{-6} : 6.0×10^{-18}.

4 SCOPE OF MEASUREMENTS AND CALCULATIONS

4.1 Measurements

Various different states of moderation were simulated by using additional polyethylene sheets, placed both in front of, and behind (in contact with), the N50 slab. Each slab is 26.4 mm thick, the other dimensions being the same as for the N50 moderator. Configurations were also adopted with cadmium sheets (1mm thick) inserted between the polyethylene, to represent geometries with an epithermal neutron flux. In each case, the configuration of additional polyethylene / cadmium is the same on both faces of the N50. These configurations are described in Table 2.

A ^{252}Cf source was used for the present intercomparison exercise. The source spectrum from ^{252}Cf is relatively well defined and representative of fission neutrons. Furthermore, the physical dimensions of typical sources are rather small, such that the source and capsule have a negligible effect on both the spectrum of spontaneous fission neutrons emitted from the source, and the absolute neutron emission rate. A ^{252}Cf source was placed at a fixed distance of 500 mm from the front face of the slab, located about the centre of the detector array, and at the midpoint of the active length of the detectors. The slab monitor was mounted at least 1 meter from the ground, in order to minimise the contribution to the count rate from neutrons which have been in – scattered from the environment, principally the concrete floor of the laboratory. A cadmium sheet covered the floor area near the detectors, to provide further protection against re – entrant epithermal neutrons. The reference geometry should be considered as the centre point of the ^{252}Cf source capsule.

Configuration	Additional polyethylene slabs (on each face of the N50)	Cadmium sheet ?	Number of polyethylene slabs between N50 and cadmium
1	0	✗	-
2	1	✗	-
3	2	✗	-
4	3	✗	-
5	4	✗	-
6	0	✓	0
7	1	✓	0
8	2	✓	1
9	3	✓	2
10	4	✓	2

Table 2. Geometry configurations. The geometry as described is symmetric on each side of the N50.

4.2 Calculations

Calculations were performed for the 10 geometry configurations described in section 4.1, using a range of nuclear data options as described below. The Monte Carlo calculations were run for sufficient time to achieve a statistical standard deviation (σ) of the order 0.5 – 1.0 %, which was expected to be considerably less than the systematic differences likely to be observed during the study. As the geometry is simple and physically quite compact, variance reduction techniques (which may introduce their own biases) are not required for this modelling.

The modelling also provided an opportunity to perform studies to explore the sensitivity to small geometry perturbations such as detector active length and polyethylene density. This work would be valuable in assessing the uncertainty in the performance of the detector, as a result of engineering tolerances.

5 MONTE CARLO CODES

MCNP^{TM} modelling is widely used as a design / calibration tool for NDA applications in both safeguards and waste management. As well as being used as a design tool to optimise the geometry of NDA assay chambers, it can greatly reduce the amount of time – consuming experimental calibration which is required, and reduce the reliance upon physical standards. For example, MCNP^{TM} simulations can be used to simulate the response of an NDA instrument to certain calibration sample types which are not directly amenable to experiment.

The ESARDA Reals prediction benchmark exercise [1, 6] was based on the use of the established Monte Carlo code MCNP^{TM} [7]. This code is used for a wide range of applications in the nuclear, defence, medical, high energy physics, and industrial applications. Probably the most widely used Monte Carlo code in general use, MCNP^{TM} has become an international standard, against which other codes are often compared. However, many other Monte Carlo codes exist, being aimed at specific application areas. For example, the Monte Carlo code MCBEND [8, 9], is aimed primarily at shielding applications, incorporating a range of physics and acceleration techniques which are tailored to these applications areas. This code is used widely in the UK for shielding calculations and assessment of radiological damage to, for example, PWR reactor pressure vessels. Similarly, the TRIPOLI [10] is not widely used for safeguards / NDA applications. Although these codes have not been routinely applied to NDA applications, this is possible, and hence there is interest for the current intercomparison exercise. Since nuclear data is generally processed to provide a uniform (compatible with different operating platforms), transportable format, it is possible to use the same nuclear data (cross – sections) with different codes. This benchmark could then allow the suitability of the codes for routine safeguards NDA applications to be assessed. After a comparison has been made with MCNP^{TM}, any special features of MCBEND and TRIPOLI could be explored to determine whether there would be any useful advantage over MCNP^{TM} in safeguards applications.

Modified versions of MCNP^{TM} have been developed, designed to simulate the complete pulse train history in neutron counting systems, as well as performing the random walk tracking of particles in the usual fashion. These codes permit a complete simulation of the pulse train, including the arrival times of events at the detectors, allowing the prediction of coincidence count rates in typical coincidence electronics, without relying on the assumptions of the classical single point model. Two such codes are "MCNP-REN" [11] which has been developed at the Los Alamos National Laboratory, and "MCNP-PTA" [12], developed at the Joint Research Centre (JRC), Ispra. These codes offer no advantage to the present exercise, as they are directed at simulation of the response of coincidence counters. However, these codes are also being tested for PNCC safeguards systems, and may also be studied in a future ESARDA intercomparison exercise.

6 NUCLEAR DATA

It was intended to explore the available neutron cross-section data sets which are available for use with codes such as MCNP^{TM}, MCBEND and TRIPOLI. Although the raw cross–section data evaluations for many elements / isotopes are the same across various evaluated cross-section libraries, there are differences in the data processing techniques used, in particular the fineness of the energy meshes used. Also, there are some well known changes to cross-sections which have occurred in later revisions of standard libraries, which result in more accurate data over certain energy ranges (notably, resonance regions).

Although one might expect that the latest release of a particular cross-section library (for example, the widely used ENDF-B series) should be used in all cases, this is not necessarily the case: it is possible that there may be bugs introduced into the later version. By comparing, say, the recent ENDF library releases which are in common use with MCNP^{TM}, one can assess whether there are any important differences (improvements) associated with the later releases, with regard to neutron detectors in NDA instrumentation. By comparing different evaluations, one can compare the accuracy of the benchmarking of the Monte Carlo modelling against experiment.

6.1 Cross-section libraries

Candidate cross-section libraries include (but are not necessarily limited to) the commonly available ENDF-B5, ENDF-B6, and ENDL85. The use of the $S(\alpha,\beta)$ thermal neutron scattering treatment is also of particular interest, as this is known to be important for problems involving thermal neutron transport.

6.2 Source spectra

There are several evaluations of the ^{252}Cf spontaneous fission neutron source spectrum, which will be of interest for the present intercomparison. It is thought that differences between the shapes of the low energy tail regions of the spectrum are likely to be particularly significant.

The published ^{252}Cf source spectra representations which have been identified for use here, are as follows:

1) Watt fission spectrum obtained from [7].

$$\chi(E) = C.e^{-\frac{E}{a}}.\sinh(bE)^{\frac{1}{2}}$$

where a = 1.025 MeV,
b = 2.926 MeV^{-1}

2) Maxwellian ISO standard spectrum obtained from [13] (defined in the range 100 keV – 10 MeV) and defined as a Maxwellian as follows:

$$\chi(E) = \frac{2}{\sqrt{\pi}T^{3/2}}.\sqrt{E}.e^{-E/T}.B$$

where T = 1.42 MeV

3) Modified Maxwellian spectrum, according to [14].
This spectrum fit is based on eight documented spectrometry measurements.
The spectrum is defined by a set of correction factors, which are applied to a reference Maxwellian:

$$\chi(E) = 0.633CF\sqrt{E}.e^{-1.5E/2.13}$$

The correction factors (CF) are given by:

Energy range (MeV)	Correction Factor, CF
0.0 – 0.25	$1 + 1.20 \times 10^{-0.237}$
0.25 – 0.8	$1 - 0.14 \times 10^{0.098}$
0.8 – 1.5	$1 + 0.024 \times 10^{-0.0332}$
1.5 – 6.0	$1 - 0.00062 \times 10^{0.0037}$
6.0 – 20.0	$1.0 \times \exp[-0.03(10^{-6.0})/1.0]$

4) Watt spectrum fit, according to 15, from which values for a and b of 1.18 MeV and 1.03419 MeV^{-1} respectively are obtained.

In the above, E is the energy in MeV, while $\chi(E)dE$ is the proportion of the neutrons emitted in the energy increment dE about E.

7 RESULTS

7.1 Measurements

The detection efficiency was measured for each geometry configuration, these results are summarised in Table 3. A detailed uncertainty study was performed (see Table 4) in order to assess the overall random uncertainty associated with these results.

Geometry	Efficiency (%)	1 sigma
1	2.381E-01	3.19E-03
2	2.175E-01	2.94E-03
3	1.569E-01	2.10E-03
4	1.020E-01	1.55E-03
5	6.361E-02	1.03E-03
6	2.405E-01	3.30E-03
7	1.943E-01	2.70E-03
8	1.511E-01	2.19E-03
9	1.006E-01	1.55E-03
10	6.229E-02	1.17E-03

Table 3. Measured efficiencies for configurations 1 - 10. The 1 sigma relative standard deviation is determined from the uncertainty budget presented below.

Source of uncertainty	Relative σ (%)
Dead time losses	Negligible
^{252}Cf position	0.79
^{252}Cf source strength	0.73
^{252}Cf source anisotropy	0.40
Room Scatter	0.50
Active Length	0.12
^{3}He fill pressure	0.09
Overall	1.26

Table 4. Systematic uncertainty budget for measurements. The σ component from random counting statistics was between ≈ 0.4 and 1.4 %, the higher uncertainties being for the more highly moderated geometries. These were added in quadrature with the overall value shown above, to produce the total uncertainties shown in the results in Table 4 and Figure 2.

The uncertainty budget presented above is based on a comprehensive analysis of all the potential uncertainties originating from the engineering tolerances in the experiment and the detector manufacture.

- The source position uncertainty arises from a combination of the uncertainty due to measurement of the source distance from the N50 slab, and the uncertainty in the exact position of the source inside the capsule. The measured variation of count rate with source - detector separation, was used to estimate the resulting uncertainty in count rate (0.79 %).
- The active length uncertainty is taken from the engineering tolerance on the anode wire length, which is 0.7 mm. This leads to a combined 1σ uncertainty for the 4 detectors, of 0.12 %. To first order, the count rate is proportional to the active length so this value can be used for the efficiency uncertainty also (in fact if the active length is large compared to the source - detector separation then the fractional efficiency increase is less than the fractional increase in active length, so this is a conservative estimate).
- The estimated uncertainty in the fill pressure is 0.14 % (0.13 % from the fill pressure and 0.03 % from the ^{3}He enrichment uncertainty), which corresponds to an uncertainty of 0.09 % in detection efficiency at 4 atmospheres (where the efficiency gain per atmosphere ^{3}He is known from experience of similar counters with different fill pressures, to be ≈ 15 %).
- The room scatter component was estimated by various methods, which all demonstrated that this is negligible at the source – detector spacing adopted. The N50 was mounted ≈ 1.6 m above the ground, and measurements with the N50 covered in Cd sheet indicated no significant difference. A power law fit to the count rate versus N50 - source separation curve, with a constant term added to allow for room scatter, suggested that the latter was close to zero, and less than ≈ 1 %. A conservative 1σ estimate of 0.5 % was thus used.

The Monte Carlo modelling methods used for this exercise assume that 100 % of the reaction products are captured in the gas, and deposit their full energy so that they appear above the discriminator threshold. In real applications, there are a number of physical reasons why this may not be exactly the case. Most importantly, wall effect losses can lead to incomplete charge deposition in the gas by one or both of the primary reaction products, if the primary event occurs near the cathode. Counting loss mechanisms such as this lead to measured detection efficiencies being lower than modelled. An estimate of the magnitude of this effect can be gained from the slope of typical counting plateaux. Typically, gradients of 1 % per 100 volts are observed, which is indicative of the counting losses due to wall effects. Further, low amplitude γ ray pileup events can sometimes give an increased signal, if the High Voltage Bias is not set to appropriately to eliminate these effects. However, usually the bias is set so that for low γ dose measurements, this is a negligible effect.

However, it is possible that this $\approx$ 1 % loss is partially, or more than, compensated by detector end effects. ^{3}He thermal neutron reactions within the "dead space" gas volume beneath the anode wire lower guard ring will, if the reaction products are directed vertically parallel to the anode, lead to some energy deposition in the multiplying region of the gas. Typically, the dead space represents a few % of the total detector volume, so that the corresponding increase in signal may be of the order of 1 %.

It would be of interest to perform some additional experiments / calculations to determine the magnitude of these effects. However, taking these two factors into consideration, it is considered reasonable for the present purposes to allow an additional 1 % contribution (1 σ) to the overall uncertainty. This leads to an overall systematic 1 σ uncertainty of $\approx$ 1.6 %, when combined in quadrature with the overall value in Table 4. This is considered to be indicative of typical uncertainties in detector geometries allowing for measurement uncertainty and engineering tolerances. It can therefore be considered as a limit to the level of agreement which can be reasonably expected, between measurement and calculation. If we allow a small contribution for counting statistics (generally several repeat runs each with a nominal precision of < 1 % were performed for each configuration), this becomes $\approx$ 2 %.

7.2 Monte Carlo results

The results for the different configurations, are shown in Figure 2. Since the participants used predominantly ENDF B6 cross-sections with different source spectra, the results presented here are therefore limited to the ENDF B6 data. No significant difference was observed between ENDF B5 and ENDF B6. The results for group B are not included, some further investigation being required.

results clearly demonstrate the importance of the S(α, β) treatment (group A showed that for the heavily moderated geometries, failing to use this treatment gives gross over estimates for the efficiency.). This finding is consistent with general industry experience, shared at the ESARDA NDA Working Group meetings.

The results show that there is a significant spread in the results from the various groups, of about the same order as the spread in values by varying the source spectrum alone. This is attributed primarily to differences in the modelling styles used. However, the systematic differences observed between the source spectra, are broadly consistent across the different groups. It is clear from the results that any preference towards a particular source spectrum is dependent on the state of moderation. It is interesting to note that in general the Watt (Froehner) spectrum [13] studied by two groups appears to give the minimum overall discrepancy and therefore would seem to be a good choice for general simulations. This is not necessarily the case for all geometries (for example, group E compared the

Froehner spectrum with the Watt and ISO 8529 results, finding better agreement with experiment for 5 geometries, poorer in 3 cases and similar agreement in the other 2 cases) and indeed some of the better agreement could be fortuitous. However it is considered to be a good general recommendation, based on the results of the present exercise.

Group H investigated the potential benefit of the in - built variance reduction techniques in MCBEND, to reduce the run time required. It was found that by using MCBEND's automatic importance generation technique, the run time required to achieve a particular statistical figure of merit could be reduced by a factor of ≈ 3. This is interesting, and suggests that these features would be worthwhile being investigated more by Monte Carlo modellers. This would be particularly useful for modelling heavily over moderated neutron counting systems.

There is no noticeable difference in performance between MCNP™ and MCBEND or TRIPOLI. This gives confidence that these latter codes are also suitable for this type of application.

The level of agreement between calculation and experiment is summarised in Table 5. The average discrepancy is typically up to ≈ 3 %, showing a tendency to increase with state of moderation. However the spread is somewhat higher, ranging from ≈ 3 - 4 % up to ≈ 10 % for highly moderating cases. This reflects the greater effects of differences in the geometry modelling / source spectrum, for highly moderated cases in which the number of collisions is high.

Configuration	Average relative discrepancy (%)	Standard deviation of discrepancies (%)
1	-3.3	4.6
2	1.2	1.4
3	2.2	3.5
4	3.1	6.5
5	5.5	9.0
6	-4.6	4.7
7	0.0	1.7
8	0.8	3.8
9	1.4	6.8
10	2.3	9.3

Table 5. Summary of observed discrepancies between calculation and experiment. The results for all participants using ENDF B6 have been used, excluding those without the $S(\alpha, \beta)$ treatment.

7.3 Monte Carlo sensitivity studies

Sensitivity studies have been performed to determine the sensitivity of the results to certain key geometry and nuclear data perturbations.

It was generally found that the effect of air scatter is negligible compared to the overall discrepancies observed, and thus is not critical for inclusion in the model. The effect was observed to be between 0 and 1 %, in the modelling performed. In practice, one should also consider the air humidity as this can greatly affect the hydrogen content; however this is anticipated to be difficult to quantify for general modelling applications and so is not discussed further in the context of the present exercise. Modelling a sphere of radius 5 m is assumed to be sufficient to include all orders of scatter which could potentially have a significant contribution to the result.

The sensitivity to polyethylene density has been studied in detail by group F for each configuration. In summary, the variation of efficiency with polyethylene density, exhibits a good fit to a straight line in each case. The relative % shift in efficiency per 0.01 g.cm^{-3} increment is obtained from the slope of the line. The results are given in Table 6. As the uncertainty in the polyethylene density is estimated to be no more than ± 0.01 g.cm^{-3} , these can be used as a guide to the likely uncertainty in the efficiency. As can be seen, this ranges from ≈ 1 to 2.5 %. Groups D and H performed similar studies for configurations 1 and 5 respectively, and found results in excellent agreement with these values. Group H also demonstrated that the "first order sensitivities" perturbation method could be used in MCBEND to produce similar results, without having to repeat the Monte Carlo run with a different density value. It is possible that a better overall fit could be achieved by artificially adjusting the modelled density. However, this is just one of the sources of uncertainty and should be considered along with the other sources identified here. The purpose of the present study is to determine the overall level of agreement that can be achieved using a model which is as close to the real physical geometry, as possible.

The sensitivity to changes in the diameter of the detector holes has also been studied by group F. The effect of increasing the hole diameter from 27 to 28 mm was found to be a general, relative increase in response of between 0 and ≈ 2 %. This gives an idea of the uncertainty introduced as a result of not knowing the hole diameter to absolute accuracy.

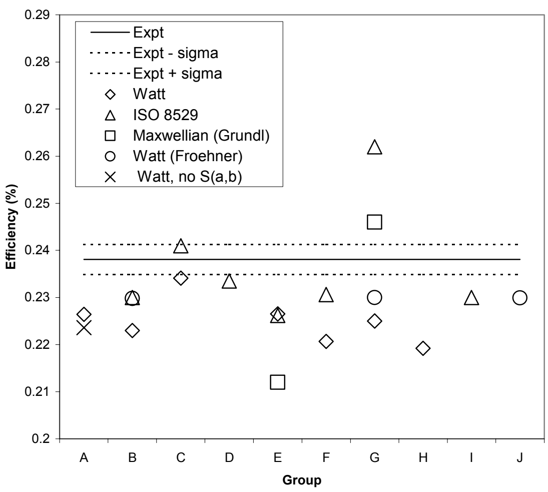
Configuration	% increase in efficiency (relative to 0.94 g.cm^{-3}) per 0.01 g.cm^{-3} increase
1	0.73
2	-0.23
3	-1.13
4	-1.84
5	-2.45

Table 6. Results of sensitivity study to polyethylene density performed by group F.

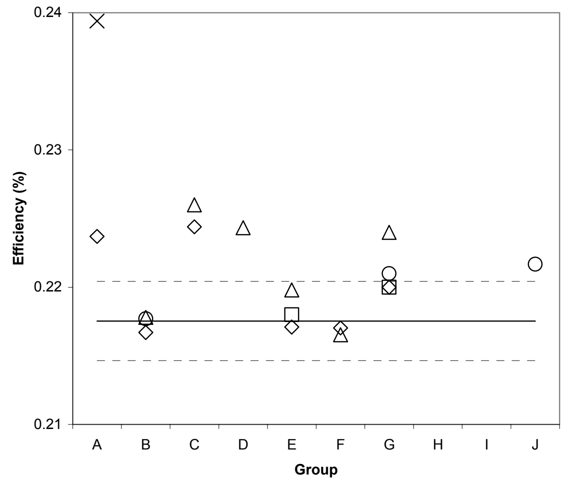
The sensitivity of response to active length was studied by group F. In fact the increase in response was found to be approximately half of the fractional increase in active length. Thus the uncertainty component assigned to the measurements (Table 4) is pessimistic.

The influence of differing neutron cross-section libraries was studied. Groups C and D found negligible difference between the ENDF B5, ENDF B6 and ENDL 85 libraries commonly available to MCNP™. Group F, however, observed little difference between ENDL85 and ENDF B5 while the ENDF B6 results were consistently lower than these, the relative difference ranging from ≈ 1 -2 % for lightly moderating geometries, up to ≈ 5 % for heavily moderated cases. The reason for this difference is not clear. However, it would be a very surprising conclusion if one were to recommend the use of anything apart from the most recent release of the ENDF B library. However, this aspect is beyond the scope of the present study and this shall not be explored further, here. It may be considered practical to use the ENDF B5 library rather then ENDF B6, since the latter does not contain cross-sections for natural elements, the natural isotopic composition having to be entered manually. However, care is required if consideration is being given to using ENDF B5 data instead of the most recent release, ENDF B6, because some data did change between these two releases (e.g. Iron).

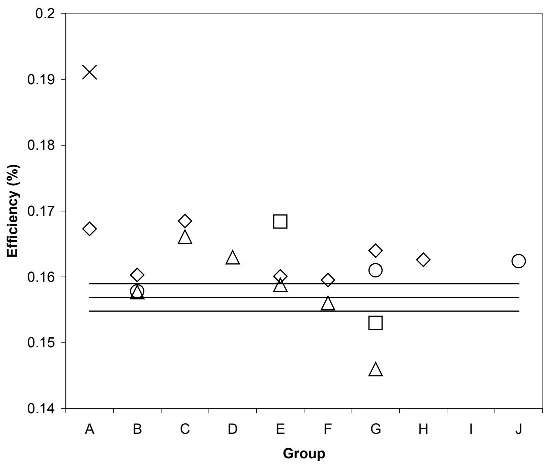
Configuration 1



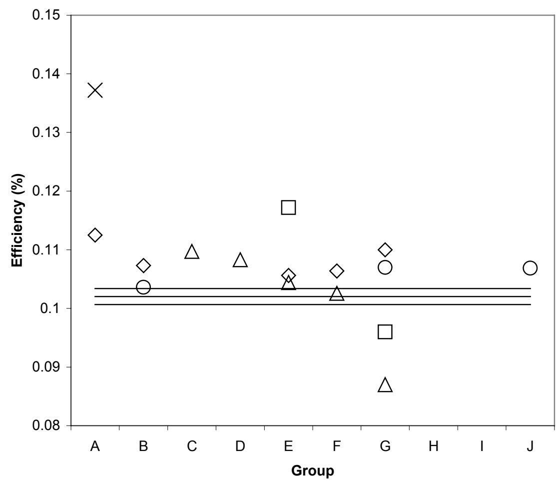
Configuration 2



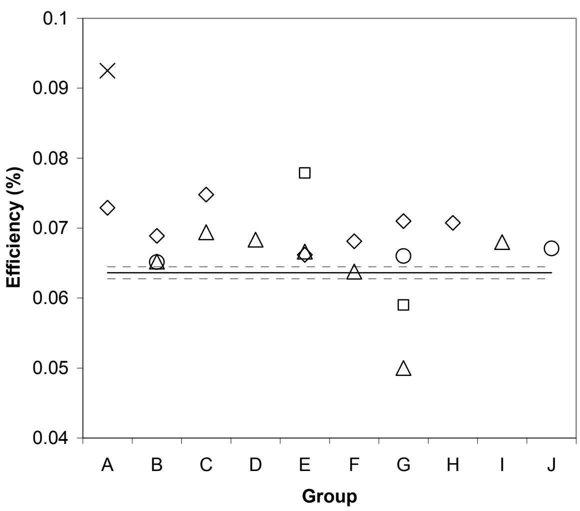
Configuration 3



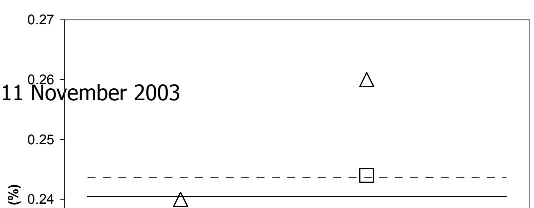
Configuration 4



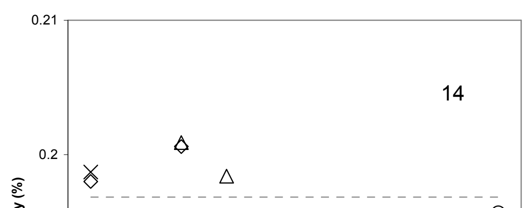
Configuration 5



Configuration 6



Configuration 7



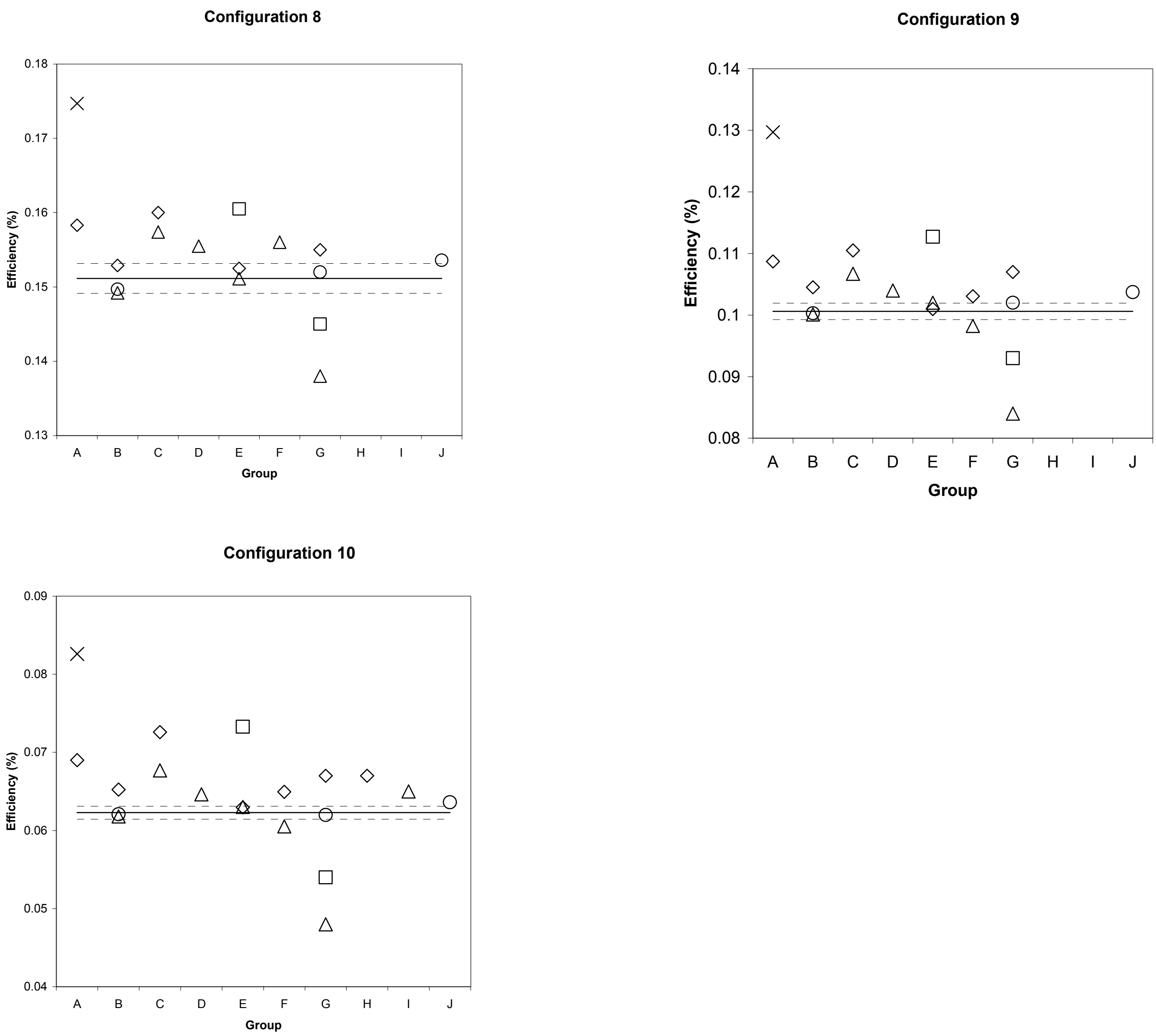


Figure 2. Comparison of calculated and measured efficiencies for the 10 geometry configurations. The calculated results shown have used predominantly ENDF B6 cross-section data sets. The measured value is shown by the solid line in each case, the dashed lines indicating 1 standard deviation limits.

8 CONCLUSIONS

The exercise has demonstrated that Monte Carlo modelling can be used to predict the Totals counting rate for a simple neutron counting geometry, to a typical level of agreement (with measurement) of ≈ 5 %, for typical lightly moderated geometries. The spread of results according to different nuclear data (principally the neutron source spectrum) and modelling styles, is also of the order of a few %, for lightly moderated geometries. For heavily moderated geometries, however, this spread increases substantially (up to ≈ 10 %), such that the influence of the nuclear data and modelling approximations are accentuated.

MCBEND and TRIPOLI have been shown to perform equally as well as MCNP^{TM} for this generic application, and the potential significant benefits of conventional variance reduction techniques have been demonstrated, even for a simple geometry such as this.

The exercise has shown some evidence to suggest that the ^{252}Cf source Watt spectrum fit according to Froehner, is a good spectrum to be used; the typical bias being minimal.

The careful experiments and comprehensive uncertainty analysis have provided a useful insight into the fundamental physics limitations to the level of absolute agreement which can be expected between measurement and calculation. We have shown that the physics uncertainties concerning largely the physics and design of the ^{3}He detectors, lead to a minimum uncertainty (1 σ) of the order of 2 % in the efficiency for this geometry. This is largely irreducible because the source strength for instance is limited by the absolute calibration of the Manganese bath method and the knowledge of the source position is limited by the size of the inner volume of the source capsule. Furthermore, if one considers the typical uncertainties in the bulk density of polyethylene, an additional component of between ≈ 1 and 2.5 % can be expected, increasing the overall uncertainty to up to ≈ 3 %. One cannot, therefore, expect better agreement than this, no matter how carefully one measures the detector dimensions, etc. The closeness of the computed results to the measured values for this Simple case benchmark exercise, are comparable to those found in the recent Reals Prediction Exercise. The Simple case benchmark is a far simpler geometry, but a wider range of nuclear data has been studied.

Current widespread practice in Monte Carlo modelling is to artificially adjust certain key parameters in the geometry model (such as the polyethylene density), in order to force very close agreement with a benchmark measurement geometry. This approach recognises the fundamental limitations posed by the uncertainties in geometry and nuclear data such as have been highlighted in this paper. It allows future studies to be directed at complex geometries such as those containing multiplying assemblies of fissile material, for which the quality of the assumed nuclear data such as the prompt and induced fission neutron multiplicity moments, is of interest.

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