Calculation of the Performance of 3He Alternative Detectors with MCNPX

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Abstract—This paper describes the techniques that are available to calculate the performance of 3He alternative detectors using MCNPX. Calculations of the performance of safeguards detectors that use 3He have been successfully carried out for many years. In the case of coincidence or multiplicity counting, specific tallies have been implemented to calculate the Singles, Doubles and Triples counting rates. The implementation of the method was done in such a way that it equates every capture in some nuclide in the detection zone with the production of an electronic pulse from the detector. This is a very good approximation for 3He detectors and BF3 detectors. However it is not appropriate for detectors such as boron-lined proportional counters, in which the fraction of capture events leading to an electronic pulse above threshold is very dependent on the geometric arrangement, in particular the thickness and composition of the boron-containing layer. This paper gives calculations of the ideal pulse height distributions to be expected from different detector types and gives values for the probability, as a function of detector energy threshold, that a neutron capture reaction will cause an electronic pulse from the detector. This is termed the electronic efficiency. This electronic detection efficiency depends very little on the energy of the captured neutron, which in most practical cases are heavily weighted towards thermal energies. It does not depend on the position of the source neutron or moderation in the sample. For cases of interest to nuclear safeguards, measurement of uranium and plutonium in specially designed detectors, the spectrum of detected neutrons is fairly constant and thus the electronic detection efficiency becomes a detector constant. The paper discusses how the electronic detection efficiency needs to be included in the calculation of Singles, Doubles and Triples, and describes proposals to improve the tallying capability of MCNPX for such cases.

I. INTRODUCTION

Simulation of neutron detector operation is an essential tool in the design and calibration of instrumentation for safeguards measurements of uranium and plutonium. Simulation and experimental work carried out in parallel improve the quality of both activities by illuminating potential problem areas. Such work has been carried out for many years in the area of neutron multiplicity counting using \(^3\)He detectors. The original work was carried out by Monte Carlo estimation of the detection efficiency, multiplication, and die-away time of instruments and the detector counting rates were subsequently calculated using a “point” model [1]. In 2003, a new coincidence calculation capability was introduced into MCNPX [2,3] to remove the need for the point model assumptions. This capability allowed the direct calculation of the detected multiplicity distribution and hence all of the correlated counting rates (Singles, Doubles, Triples…). It required associated changes so that the correct spontaneous fission multiplicity distribution was used for the source and the correct multiplicity from induced fission was also included. (Earlier versions of MCNP and MCNPX used only 2 values for the number of neutrons emitted from induced fission — the integer values immediately above and below \(\bar{\nu}_c\) (the mean number of neutrons per fission), weighted to give the correct value of \(\bar{\nu}_c\).) This new coincidence capability accounted for all of the positional variation of efficiency and multiplication, which was previously difficult to include. (One early approach to this problem was to break the sample into many pieces, for each of which the point model assumptions would hold. This worked reasonably well but was quite laborious.) However, one very important assumption that was made in implementing this new capability was that each capture in the reaction material (e.g. \(^3\)He) led to a detected pulse in the counting system. This is a very good assumption when the reaction material is in the gas phase (\(^3\)He, BF3) but unfortunately is not valid in cases where the reaction material is solid and the reaction products have to escape from the material and deposit their energy into a gas for detection. If the use of non-\(^3\)He systems is to increase in the safeguards and nuclear materials accountancy areas, it is important that suitable calculational tools and methods are developed for appropriate simulation.

II. MCNPX METHODS

Most of the neutron detector modeling carried out with MCNPX (and MCNP) for safeguards instrumentation used only neutron transport. Neutrons were started from spontaneous fission and \((\alpha,n)\) reactions. These were transported through the material and fission and absorption reactions were included. At the end of the history the number of reactions with, for example, \(^3\)He was counted. The number of \(^3\)He reactions per source neutron was taken as the product of detection efficiency and neutron multiplication. The number of reactions was normally calculated with an F4 (track length) tally using a flux multiplier to give the reaction rate. With the 2004 modification to the F8 tally the number of capture reactions in the detection material was counted directly. The two methods give excellent agreement for the total capture rate. The F8 capture tally had the desired advantage that the complete observed multiplicity distribution could be determined with experimental parameters such as.
pre-delay and gate without the use of point model assumptions.

A. Using the Current MCNPX Version

In order to calculate the Singles, Doubles, Triples (etc.) rates from boron-lined detectors without modification of MCNPX itself, there are (at least) 2 possible methods. One method is to calculate the detection efficiency and die-away time, as was done before the introduction of the F8 capture tally. Instead of calculating the initial reaction rate however, it is necessary to calculate the number of events that deposit sufficient energy to create a pulse. With MCNPX it is not possible to follow the multiplication of the charge caused by the electric field in the tube and so some approximations have to be made. The second method uses the concept of “electronic efficiency” that is a factor that affects some fraction of all pulses. The first method is valid for all cases where the point model is valid. The second method avoids the limitations of the point model with respect to positional dependence of efficiency and multiplication.

Both methods require that MCNPX estimates the energy deposited in the detecting gas. In addition to tracking neutrons, this requires tracking the charged particles that result from the capture reactions and determining the amount of energy deposited in the detecting gas. MCNPX offers a number of ways to perform this calculation. As the current version MCNPX cannot calculate the transport and multiplication in the detector as a function of the electric field, we will be limited to an estimate of the effect of this transport and the subsequent processing in the preamplifier. For example the pulse height spectrum of a 3He tube measured with a long time constant shows a large narrow peak corresponding to 762 keV of energy deposited but a more practical setup with a faster shaping time changes the observed pulse height spectrum considerably, because of variations in the position and orientation of the initial ionization. These effects will be important if we are to consider the effect of the electronic threshold on the observed counting rate.

How to calculate the pulse height

There are number of different methods that can be used to calculate the energy deposition following a nuclear capture reaction in a detector. There are a number of MCNPX options that can be used with each method and these can be affected by the version of the code as well as the cross-section data files that are used. In general, the later the version of the code, the more flexible are the options. In order to determine the deposited energy it is necessary for the code to create the charged reaction products. Generally, MCNPX expects the description of reaction products to be contained in the cross-section files. There are two disadvantages when relying on this method. The first is the quality of the cross-section data – not all files have a description of these products. Secondly it is important in most cases that the tracking of all the products from one reaction is done in such a way that the charge deposited by each particle is summed to give the overall charge deposition. The way MCNPX handles the information from the cross-section file does not always ensure that this is the case. For these reasons a kinematic model of various interactions of detector importance was added to the code [4]. This model “Neutron Capture Ion Algorithm”, NCIA, can be invoked to produce the reaction products for a few specific reactions, which are then tracked in the appropriate way. This allows us to obtain the desired result for reactions with 3He, 6Li and 10B. In the original implementation (MCNPX 2.6.0) if there were data in the cross-section file, these took priority over the use of this algorithm. This resulted in different behavior when using ENDF/B-VI data and ENDF/B-VII data, for example, depending if particle production data existed in the file. In a later version (MCNPX2.7d) it became possible to override this default and choose either cross-section data or the model calculation.

3He Energy Deposited

We will start with the calculation of the amount of energy deposited by neutron interactions in a 3He gas detector. In the methods described above in traditional modeling, in order to calculate the 3He capture rate it was only necessary to model the detector with the correct atom density of 3He. Now that we will be tracking the secondary charged particles, it is necessary to model all significant contributors to the stopping power of the gas for those particles. We will take the case of a detector with argon included in the gas mixture. Argon is included in many tubes in order to reduce the path length of the charged particle tracks and thus reduce the wall effect. If we take a “4 atmosphere” (= 4 atmospheres of 3He) tube with 23% atom fraction of argon we obtain a 3He density of 4.991 × 10⁴ g/cm³ and a total density of 2.028 × 10⁻³ g/cm³. MCNPX has an F8 pulse height tally capability, but whenever this is used in a neutron transport case, a warning is given that F8 tallies are unreliable for neutron cases. This is because these tallies must be used with care. It should be noted that it is possible to produce a tally with MCNPX in a way that seems to work but gives misleading information about the amount of energy deposited. For 3He and BF₃ detectors, for example, the basic F8 pulse height tally does not give the correct spectrum of energy deposited by the two charged particles and scores them separately. This results in an incorrect tally distribution. Fig 1 shows the results obtained for the proton energy deposition (F8:h), the triton energy deposition (F8:t) and the energy deposition of both particles (F8:h,t). However the correct energy deposition spectrum can be calculated by following the MCNPX-recommended procedure, in which the energy deposited in the gas by each particle is tallied separately and then combined using the F8 phl (pulse height light) option. An extract from the relevant MCNPX input is given in Fig 2. This results in the correct spectrum of energy deposited by the combined particles as shown in Fig 3. This procedure can also be used to get the energy deposition by one of the particles, if desired.
higher pressure gas allows the charged particles to deposit all of their energy in the gas, whereas in the lower pressure gas they deposit only part of their energy. These features are important for setting the electronic threshold and for determining the effect of gamma dose on the tube. Fig 5 shows the same data for a 2μm boron carbide layer. This shows how the thicker layer smoothes out the spectral features. One of the potential problems of modeling this type of tube is that not only is the composition of the reacting layer often proprietary, but the method of application and thus the likely variation in thickness is also not known. It is likely however that by comparing pulse height spectra with calculations it will be possible to obtain the effective thickness of the layer which can be used in subsequent calculations.

Fig. 1. Basic F8 tally showing incorrect energy deposited in ³He detector

F6: h 6 $ cell 6 is the gas
sd6 1
f6: t 6 $ no energy bins needed
sd16 1
fC8 Sum of proton and triton
F8: h 6 $
ft8 phl 2 6 1 16 1 0
e8 0 1e-5 25e-3 75e-3 100e-3 155i 4

Fig. 2. F8 PHL example input

Fig. 3. F8 PHL tally showing correct energy deposited in ³He detector

Fig. 4. Spectrum of Energy Deposited in boron-lined detector (0.75µm B₄C layer)

Fig. 5. Spectrum of Energy Deposited in a boron-lined detector (2μm B₄C layer)

It should be noted that the shape of the curve of energy deposited is not the same as the pulse height spectrum seen in practice. The electronics has a large effect in some cases because of the different shapes (rise times) of the current pulses produced by charged particle tracks with different orientations. If long shaping times are used, it is possible for the measured pulse height spectrum to approach the energy deposited curve, but under typical operating conditions, with a fast shaping time, the pulse height spectrum is significantly different. In order to interpret the results for particular threshold values it is necessary to consider these effects. The present calculations also do not take into account the effect of gamma dose rate at the tube.

Point Model

The detection efficiency is simply given by the number of counts above the energy threshold divided by the source strength (after correcting for neutron multiplication). In the point model there is only one value for the efficiency, which is used for both spontaneous fission neutrons, induced fission neutrons and (α,n) neutrons. In many sample of interest (in particular, oxides) the average energy of the (α,n) neutrons is fortuitously close to the average energy of spontaneous fission neutrons. Thus the efficiency is measured using an F8 PHL tally to determine the pulse height spectrum and applying a fixed threshold to determine the number of events detected. The dieaway time was traditionally calculated by making a tally of the reaction rate as a function of time after the spontaneous fission event. This works well for detector
Neutron well counters are designed to have a detection efficiency that is independent of energy and position and so that fulfills the point model assumptions reasonably well. The following is an example of calculating the counting rates of the Epithermal Neutron Multiplicity Counter (ENMC) [5]. This is a $^3$He-based system and so both the point model and the existing F8 capture tally are applicable and so a comparison between the two methods can easily be made. Table I shows the parameters obtained from an MCNPX run for a plutonium oxide sample in the ENMC.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Point Model Calculation</th>
<th>Coincidence Tally Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutron Multiplication</td>
<td>1.1089</td>
<td></td>
</tr>
<tr>
<td>Efficiency × multiplication</td>
<td>0.7019</td>
<td></td>
</tr>
<tr>
<td>Dieaway time</td>
<td>21.74 µs</td>
<td></td>
</tr>
<tr>
<td>Gate fraction (1.5, 24µsec)</td>
<td>0.6239</td>
<td>0.3310 cps</td>
</tr>
<tr>
<td>F8 capture tally (1.5, 24µsec)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Doubles/source neutron</td>
<td>0.3350 cps</td>
<td></td>
</tr>
</tbody>
</table>

In order to determine the numerical value of the electronic efficiency it is necessary to model the behavior of the charge particles, as above, and produce the energy deposition spectrum. Fig 6 shows the electronic efficiency calculated by summing the pulse height spectrum above a fixed threshold for those cases in Fig 4 and Fig 5 above. These results can be used to give the effective counting efficiency for a particular threshold. Note the steepness of the curve. In contrast to the $^3$He (and BF$_3$) case where the counting efficiency is insensitive to the threshold setting, in these detectors, the counting efficiency changes rapidly as the threshold (or equivalently the gain) of the system changes. This implies that it will be difficult to reach the same level of count rate stability with this type of detector as with $^3$He.

Care should be taken when estimating the electronic efficiency from the spectrum of energy deposited even when the F8 PHL tally is used correctly. For a source of single neutrons, without neutron multiplication, it is possible to produce the correct spectrum. However for spontaneous fission sources and cases with induced fission, it should be noted that the PHL tally gives the energy deposited per history rather than per neutron. This can lead to important differences in the shape of the spectrum, with fewer entries and some high values of energy deposited. The modeling also has to take into account the true energy distribution of the neutron flux at the detector.

Electronic Efficiency
If we define the “electronic efficiency” as the number of events that deposit sufficient charge in the detecting gas per capture event in the detection material, then this number is very close to 1.0 for $^3$He and BF$_3$. This assumes that these detectors are operated under good conditions: on the plateau and with no gamma interference. The electronic efficiency will be significantly less than 1.0 for boron-lined devices, depending on the thickness and composition of the deposit. For a detector operated under a fixed set of conditions this electronic efficiency is effectively constant. It depends on the detailed behavior of the charged particles in the detector as well as the subsequent electronic processing, but these details are constant in most detector designs of safeguards interest. The electronic efficiency does not depend on the position of the source neutron or moderation in the sample and is essentially independent of the initial neutron energy, because the neutrons are at or close to thermal energy when they react in the detector. This electronic efficiency reduces the total number of counts by a fixed proportion, reducing the overall counting efficiency. Therefore in calculating the counting rates with the point model we would expect to have to reduce the MCNPX-calculated efficiency by this fraction. It would appear linearly in the Singles count rate, as the square in the Doubles count rate and the as cube in the Triples count rate and so on. This electronic efficiency is dependent on the type of detector tube defined by layer composition and thickness, filling gases, dimensions and processing electronics and the neutron spectrum. In conventional gas detectors, a capture reaction has a high probability of creating a pulse. In the boron-lined case the probability of producing a pulse increases with increasing neutron energy because higher energy reaction products are produced and these have a higher probability of escaping from the layer and depositing more than the threshold energy in the gas.
B. New MCNPX Developments

Although the above methods allow coincidence calculations using the point model, this is not a convenient approach in many cases. Therefore in order to allow the existing F8 capture tally to give results in more complex cases, MCNPX has been modified so that the initiating event that leads to a multiplicity contribution is not a capture in a particular nuclide, but the deposition of an amount of energy above a threshold. This capability is available in an alpha test version of the code. The modification allows the use of the F8 capture tally with an additional keyword “EDEP” (for energy deposition) that then allows the use of two additional parameters, tally number and threshold. The tally number refers to a separately defined tally that should be used to determine the energy deposited in the cell of interest. This could be an F6 or *F8 tally for both reaction products combined. When the amount of energy deposited in the cell (per neutron branch) is greater than the threshold value, the coincidence tally analysis is launched (as was done previously when a capture occurred in a nuclide of interest). The gate keyword, which specifies the predelay and gate width is still allowed.

As an example of the tallies obtained with this new version, Table II shows the results for boron-lined tubes with reacting layers of 0.2μm, 1.0μm and 2.0μm of boron carbide. The detector model included many tubes and a plutonium sample was used as the source of neutrons. The spectrum of neutrons on the tubes is not the pure thermal distribution that was the case in Figs 4, 5, and 6. The normal capture tally was used to determine the factorial moments of the 10B capture case in Fig 4, Fig 5, and Fig 6. The normal capture tally was on the tubes is not the pure thermal distribution that was used as the source of neutrons. The spectrum of neutrons detector model included many tubes and a plutonium sample layers of 0.2μm, 1.0μm and 2.0μm of boron carbide. The electronic efficiency has to be calculated taking into account the energy deposited by the charged particles escaping into the detector.

arises because, in this calculation, the energy deposited must be above 0.1MeV to be counted.

Secondly, the electronic efficiency for each case was determined. This was calculated by the ratio of the first moments of energy deposition tally in the gas and the capture tally in the boron layer, the square root of the ratio of the second moments and the cube root of the third moment. The results are very consistent as calculated from the different moments with variations of 0.2% or less. This confirms that the notion of electronic efficiency can be calculated and applied to the moments of the conventional capture tally (calculated in the reacting layer). The values in Table II have been obtained with a very early version of the code. Significant further testing and validation are required.

(In the modifications made to the code for this new capability, the problem of the direct F8 tallies on the energy deposited by the individual and combined charged particles (Fig 1) has been solved and the spectrum of energy deposited can be calculated directly.)

III. Conclusion

The alternative detectors present challenges when it comes to calculation of neutron coincidence counting rates. The specialized neutron coincidence tallies in versions of MCNPX (2.7e and earlier) were designed to be used with detector types such as 3He or BF3 gas detectors in which a capture reaction has a very high probability of causing a pulse in the detector. In other types of detectors, where this is not the case, there are other calculational methods available. One method is to calculate the detection efficiency, neutron multiplication and gate utilization factors (from the time behavior) and use the point model equations to calculate the counting rates. If necessary the calculation can be done independently for small subsamples, for each of which the point model holds. For boron-lined detectors, for example, the neutron detection efficiency has to be calculated taking into account the energy deposited by the charged particles escaping into the detector.
gas volume and comparing this with some electronic threshold. The ratio of detected pulses to capture reactions, the ‘electronic efficiency’ can be calculated from the spectrum of energy deposited in the detection gas. This factor can be combined with the coincidence capture tally to estimate Singles, Doubles and Triples (etc.) counting rates in the detector without requiring the point model assumptions. This method requires separate energy deposited tallies to be used.

A new version of MCNPX is under development, in which the coincidence tallies are based directly on energy deposited above a detector threshold. This would be the simplest way to directly calculate Single, Doubles and Triples counting rates without use of the point model assumptions. This capability should facilitate coincidence calculations for many different detector types, including boron-lined detectors and scintillators.

REFERENCES