AN ABSTRACT OF THE THESIS OF

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Past weapons production activities have resulted in mass quantities of trans-uranic waste being buried in drums at several sites in the United States. In an effort to relocate these waste drums to more permanent storage sites, Fluor Hanford has begun characterizing their contents to ensure compliance with various shipping and storage requirements. Non-destructive analysis techniques are regularly employed, among them passive radiation detection using a Canberra Gamma-Energy-Analyzer germanium detector vault. Necessary strict legal tolerances require strong quality assurance. The detectors are frequently calibrated in the traditional method with check sources, but it would be advantageous to have an estimate of system minimum detectable activity (MDA). However, any estimate is complicated by the fact that sources are distributed stochastically in the waste drums.

In this study, a method was developed to predict system detector efficiency for a variety of detector configurations and drum fill materials and calculate MDA based on these efficiencies. The various system designs were modeled in Monte Carlo N-

Particle Code, version 4b, to determine photopeak detection efficiency. An external code written in C programming language was used to randomly assign between one and 20 sources to volumetric regions of the waste drum. Twenty simulations were performed for each design and drum fill material combination, each time redefining the stochastically distributed source. This provided a normally distributed spectrum of 20 efficiencies for each situation. From this, mean and lower 95% confidence limit efficiencies were used to calculate MDA. The patterns among the results were then compared with values predicted by the MDA formula. Finally, an examination was made of the impact on the MDA of the system's true design in the case of single or multiple detector failure.

The results indicate that this method of estimating minimum detectable activity, although costly in computing time, provides results consistent with intuitive and calculated expectations. Future work would allow easy calibration of the model to measured efficiency results. Used in coordination with physical experiments, this method may eventually prove useful in benchmarking system performance and accurately ensuring reliable waste drum characterizations.

Monte Carlo MDA Determination
for Waste Drum Sources

by

Matthew A. Buchholz

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Matthew A. Buchholz, Author

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Monte Carlo MDA Determination
for Waste Drum Sources

ABSTRACT

Past weapons production activities have resulted in mass quantities of transuranic waste being buried in drums at several sites in the United States. In an effort to relocate these waste drums to more permanent storage sites, Fluor Hanford has begun characterizing their contents to ensure compliance with various shipping and storage requirements. Non-destructive analysis techniques are regularly employed, among them passive radiation detection using a Canberra Gamma-Energy-Analyzer germanium detector vault. Necessary strict legal tolerances require strong quality assurance. The detectors are frequently calibrated in the traditional method with check sources, but it would be advantageous to have an estimate of system minimum detectable activity (MDA). However, any estimate is complicated by the fact that sources are distributed stochastically in the waste drums.

In this study, a method was developed to predict system detector efficiency for a variety of detector configurations and drum fill materials and calculate MDA based on these efficiencies. The various system designs were modeled in Monte Carlo N-Particle Code, version 4b, to determine photopeak detection efficiency. An external code written in C programming language was used to randomly assign between one and 20 sources to volumetric regions of the waste drum. Twenty

simulations were performed for each design and drum fill material combination, each time redefining the stochastically distributed source. This provided a normally distributed spectrum of 20 efficiencies for each situation. From this, mean and lower 95% confidence limit efficiencies were used to calculate MDA. The patterns among the results were then compared with values predicted by the MDA formula. Finally, an examination was made of the impact on the MDA of the system's true design in the case of single or multiple detector failure.

The results indicate that this method of estimating minimum detectable activity, although costly in computing time, provides results consistent with intuitive and calculated expectations. Future work would allow easy calibration of the model to measured efficiency results. Used in coordination with physical experiments, this method may eventually prove useful in benchmarking system performance and accurately ensuring reliable waste drum characterizations.

INTRODUCTION

BACKGROUND

Radioactive waste has been a growing problem since large scale weapons production in the 1940s during the Second World War. The low priority and lack of technology for effective permanent disposal resulted in the waste being placed in steel drums and buried at temporary storage sites such as Hanford, Washington, and Savannah River, South Carolina. Continuing political and financial struggles have turned these "temporary" storage sites into long term commitments while a resolution is sought. The DOE Hanford site in Washington has large quantities of these radioactive waste drums buried in various locations on the reservation. The contents of these drums range from latex gloves laced with radioactive dust to solutions of plutonium nitrate from past extraction processes. With the advent of better facilities and states willing to house waste, private companies are regularly contracted to characterize each drum's contents with the end goal of relocating the thousands of currently buried drums to permanent storage sites.

Characterization employs a wide range of non-destructive analysis (NDA) techniques, including x-ray imaging, neutron interrogation (diffraction and activation), and passive radiation detection. Of these methods, radiation detection is perhaps the most valuable for several reasons. First, no additional radiation fields are generated. Second, the technologies are well-established and easily maintainable. Finally, it is primarily the radioactive content of the waste drums that preclude shipment and storage.

THE CANBERRA GAMMA-ENERGY-ANALYZER

Fluor Hanford, one of the primary contractors at the Hanford site, conducts characterization and shipment operations at the Waste Receiving and Processing (WRAP) Facility. The WRAP Facility uses a system called a gamma-energy-analyzer (GEA) vault designed specifically for drum characterization through radiation detection. The GEA system is a Canberra designed steel enclosure (**Figure 1**). Steel drums (55 and 80-gallons) are loaded by conveyor onto a rotating, lifting platform. Once inside, four high-purity germanium detectors and two low-energy germanium detectors take passive radiation measurements as the drum rotates at various heights. The output energy spectra are analyzed to identify the isotopes and amounts present in the drum, thus characterizing the types and amounts of radioactive substances. The vault also includes four europium-152 sources that are used to gauge density of the drum contents based on attenuation of the photons through the waste drum.

Figure 1. Photograph of Canberra GEA system at WRAP Facility.

Necessary strict legal tolerances require strong quality assurance. The detectors in the GEA system are frequently calibrated in the traditional method with check sources, and the detection results are double checked manually. However, little has been done to determine the minimum detectable activities (MDAs), i.e., the smallest amount of radioactivity that would still be detected by the system. Knowing the minimum detectable activity of the system would provide key reassurance in the NDA characterization process. It could be used as certification both of the system's abilities and, consequently, conclusions that a given drum has no measurable activity of a given isotope.

MDAs are easily calculated for most detection systems, but the stochastic (random) nature of the source distribution in the waste drums makes this unusually difficult. There may be anywhere from zero or few to tens of sources in any given waste drum. Additionally, the sources each may be at any height and radial position within the drum.

This study establishes a method for determining GEA minimum detectable activities using computer simulation to predict detector efficiencies with stochastically distributed sources. The effect of varying the number of detectors (one through five) and drum fill materials is examined, as well as what happens to the current Fluor Hanford system MDA if one or more detectors fail.

ORIGIN OF MDA

Minimum detectable activity arises from the statistical nature of radiation decay. While radionuclides decay at known rates over extended times, the true number of decays within any given time interval is unknown. However, with large numbers of decays, this rate can be shown to follow a Poisson distribution around the "true" decay rate, which, at high count numbers, can be approximated as a normal distribution. Therefore, one can never predict with absolute certainty how many decays will occur in a given time; only define the probability of observing a certain value.

Still, it is necessary to be able to conclude whether or not radioactivity is present. To do this, a threshold count rate must be established such that the possibility of a Type I (false positive) or Type II (false negative) error is controlled. A Type I error results from normal fluctuations in the background count rate exceeding a threshold (L_C), falsely indicating the presence of activity. A Type II error results if fluctuations in the gross counts from a source (L_D) fell below the threshold, falsely indicating the absence of activity.

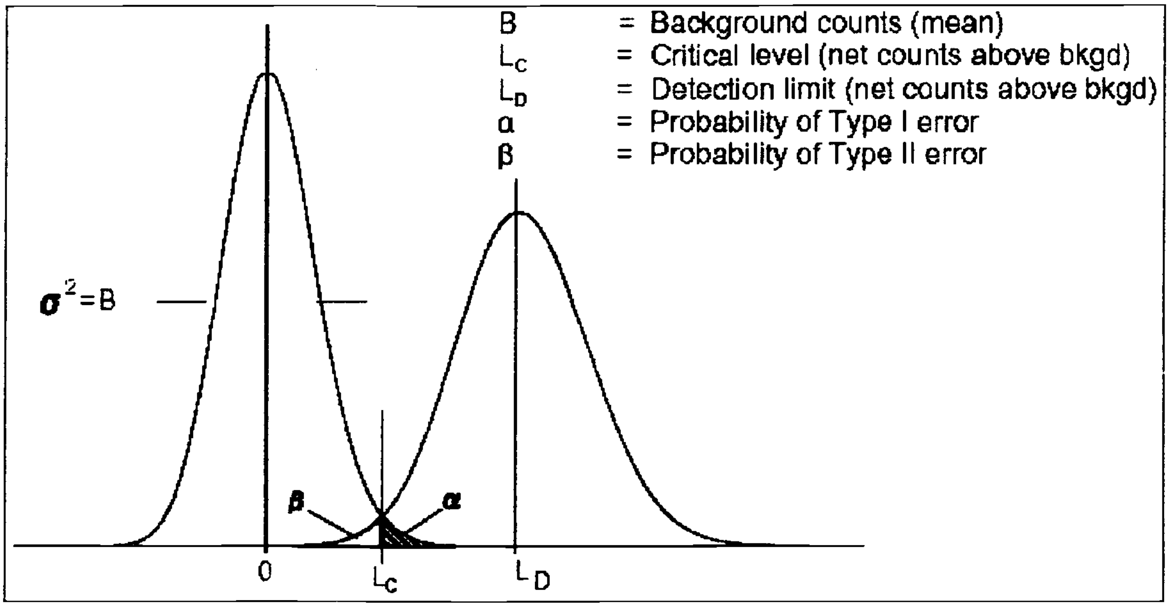

Figure 2. Diagram of background and source variations.

Defining a value α as the acceptable risk of a Type I error and a value β as the acceptable risk of a Type II error (**Figure 2**), Turner (1995) demonstrates the derivation of the formula

$$\boxed{MDA = \frac{(K_\alpha + K_\beta)\sqrt{2N_{bkg}}}{efficiency * time}}$$

where $\mathbf{N_{bkg}}$ is the measured background counts in ***time***, and $\mathbf{K_\alpha}$ and $\mathbf{K_\beta}$ are the corresponding number of standard deviations from a normal distribution mean to give one-tailed confidences of α and β. ***Efficiency*** is the ratio of counts recorded by the detector per nuclear decay due to the geometry of the system and inherent detector properties. Taking one-tailed confidence values of $\alpha=\beta=0.05$ gives $\mathbf{K_\alpha}=\mathbf{K_\beta}=1.65$ and the resulting formula for MDA at the 95% confidence level:

$$\boxed{MDA = \frac{4.65\sqrt{N_{bkg}}}{efficiency * time}}$$

Note that, since background count rates are easily recorded, determining the MDA of the Canberra GEA system depends primarily on finding the efficiency of the detectors in each geometry of interest. Consequently, efficiency is the primary measurement of interest in this study.

METHODS

MCNP

One of the primary computer simulation codes used for stochastically modeling radiation transport is Monte Carlo N-Particle Transport code (MCNP) developed by Los Alamos National Laboratory. Originally designed to perform criticality assessments of nuclear bomb designs, MCNP has since been adapted to simulate photon and electron transport. Stochastic simulation, such as in MCNP, differs from deterministic methods in that, rather than solve radiation transport equations for explicit values, particle interactions are randomly chosen from defined probability distributions.

MCNP is ideally suited to the problems posed in this study for many reasons. The probabilistic nature of the source sampling coincides with the waste drum source variability. It is useful for simulating complex geometries that inherently lose detail if described in sufficiently solvable discrete terms, such as for a deterministic calculation.

MCNP has built in automatic tallies, one of which mimics a detector energy spectrum. These tallies are normalized per starting particle, essentially providing a built-in efficiency measurement. For each tally, the estimated relative error is automatically calculated (defined as the estimated standard deviation as a percentage of the tallied value). Additionally, there are internal coding options to reduce the variance of the tallies without having to run large numbers of particles at the cost of tremendous computing time. (Briesmeister, 1997)

The Monte Carlo Method

MCNP simulates radiation transport by tracking particle life histories. A simulated environment is defined by the user in terms of 2-dimensional surfaces, 3-dimensional volumes, and defined probability distributions. A particle is tracked from birth, through interactions chosen from the probability distributions, until its eventual death, or absorption. Each secondary particle generated along the way is saved in memory and tracked through its own life history afterward. MCNP keeps running tallies of interactions and energy depositions and reports the totals in an output file. As larger and larger numbers of particles are simulated, the statistical certainty in the tally grows stronger.

Support of MCNP Use for Efficiency Measurements

The use of MCNP for determining germanium detector efficiencies is nothing new. A wealth of literature and experimental data is available validating this particular use and its achievable accuracies.

Dr. Fred Bronson of Canberra Industries, the company that produces the GEA system, wrote several papers regarding mathematical calibration of germanium detector efficiency. The first (Bronson & Young, 1997) addresses the general need to replace source-detector calibrations with less expensive, more adaptable mathematical models. MCNP use is discussed, and the data supports efficiency accuracies of 15% or greater compared to live-source measured data. Canberra had sufficient trust in the simulated efficiencies to base their In-Situ-Object-Counting-System (ISOCS) software on the MCNP characterizations.

Another paper by Dr. Bronson (Bronson & Wang 1996) is an investigation specifically of MCNP use for germanium detector efficiency calibrations. Coaxial germanium detectors are simulated in a variety of source-detector geometries. The simulations include a Canberra GEA system such as the ones at the Fluor Hanford facility. Additionally, multiple drum fill materials are simulated to examine attenuation effects. Accuracies were reported within 10% of experimentally measured values for a variety of geometries. Data appeared limited, however, on variations of the GEA design with respect to the number of detectors or their position within a geometry, and no discussion is made of stochastically distributed sources.

Ludington and Helmer (1999) similarly studied the use of Monte Carlo calculations for determining germanium detector efficiencies. While their study used a CYLTRAN Monte Carlo code as opposed to the Los Alamos MCNP, there are many valuable insights. A simple yet effective simulated detector design was used, and a report made of parameter sensitivity effects. For instance, dead-layer thickness was shown to have minimal or no effect. The only variable that appreciably changed results was crystal length. This is supportive of the assumption that exact physical accuracy is not essential in many of the finer geometry details. It is the size of the crystal active-area that has the greatest impact. Most importantly, shielding materials around and behind the detector are unimportant since reflected photons will not deposit at the full energy peak. This assumption was carried over to this study. This significantly reduces model complexity and simulation run time.

A study by Fehrenbacher, Meckbach and Jacob (1996) additionally supports the accuracy of a simplified detector design using MCNP version 4b, the same version of MCNP used in this study.

Rodenas, Martinavarro and Rius (1999) concluded that accuracies of germanium detector efficiencies are achievable to around 10%. The study included shielding effects and radial displacement of the source from the center axis of the detector.

MCNP MODEL

The high-purity germanium detectors used in the GEA system were reproduced in MCNP according to Canberra's published specifications and factory schematics. It is neither feasible nor necessary to reproduce every intricate detail. However, the model complexity was consistent with that in the Ludington and Helmer (1999) study. All simulated detectors were based on Canberra model GC2020 standard-electrode high-purity germanium detectors (SEGEs) used in the Fluor Hanford GEA system.

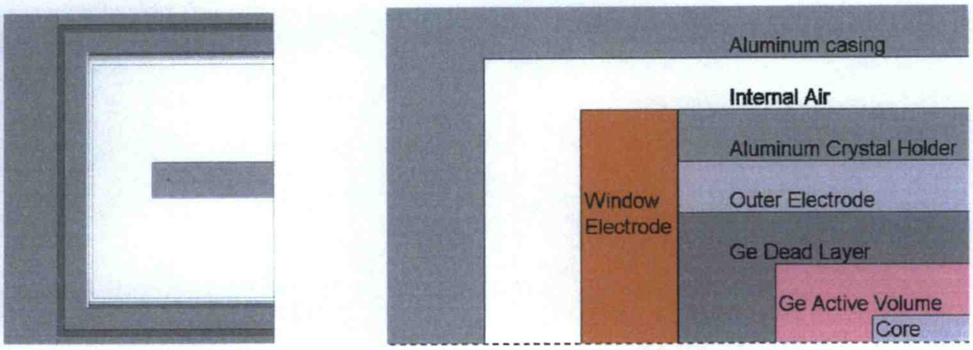

Figure 3. MCNP detector plot and half cross-section.

As illustrated in **Figure 3**, each simulated SEGE includes the aluminum casing, crystal holder, germanium equivalent window and outer electrodes, core signal contact, dead layers, and crystal active area. The active area consists of a cylinder 55 mm in diameter and 42 mm long, minus the 8 mm diameter core contact cylinder penetrating 27.5 mm from the end.

The vault design is much more forgiving in terms of simplicity than the detector. The MCNP model simulates an air-filled vault with a 55 gallon steel drum resting on the floor. The right wall containing the detectors is modeled as the appropriate thickness of steel with openings for each detector well. Immediately internally adjacent the wall is the SEGE shield. In reality, this is a steel shield that can slide in front of the SEGE wells during high count rates to prevent swamping the detectors. In the simulation, the shield volume can be filled with either air or steel to allow calculations both with and without the shield in place. The remaining five walls of the vault have no dimensional thickness, and are essentially voids into which photons are absorbed and no longer tracked.

On the wall opposite the detectors are the four europium collimation tubes. As previously described, the europium sources are slid into place when needed to gauge attenuation, i.e. density, of the drum contents. While these tubes are always present in the MCNP geometry, the europium sources can be "deactivated" by not being entered in the model source term.

In reality, the GEA system is capable of moving the drum vertically while rotating within the vault. This allows for the detectors to view the drum at various heights and make a determination of source locations. MCNP cannot model geometrical movement, and this spatial information is irrelevant to this study of

MDA versus number of detectors. The simulation thus treats the drum as rotating while placed at floor level. MCNP efficiency simulations of a GEA system by Canberra's own staff (Bronson & Wang 1996) used a similar approach, without stochastic source distribution, and achieved good results.

Ludington & Helmer's work in 1999 simplifies the necessary vault geometry with several assumptions. First, coherent (Thomson) scatter is negligible in the energy range and low angles of interest. Second, incoherent (Compton) scattered photons would not deposit at the full energy peak even if they survived to the detector. These simplifications are the basis for the absence of the five walls as well as the housing apparatus behind each SEGE.

MULTIPLE GEOMETRIES AND FILL MATERIALS

While designing a methodology for determining MDA of stochastically distributed sources, there is an opportunity to study the change in system MDA for varying numbers of detectors. This will allow the system to be designed for a desired MDA without the cost and complication of excessive detectors. To this end, geometries were constructed for 1,2,3,4, and 5 detector versions (**Figure 2**). In each case, the detectors are equally distributed over the axial height of the drum.

An additional study is made of the effect of detector failure on MDA in the GEA system as it exists at Fluor Hanford. This sixth, "true" geometry actually in use is slightly different from the equally distributed detector geometries in that it is meant to allow for spatially locating the source within the drum. The true system has four detectors placed such that, when the drum is at floor level, the uppermost detector overshoots the top of the drum. Likewise, when the drum is completely raised, the lowest detector undershoots the drum.

A simulation was made of this true geometry so that MDA calculations can be made with data lacking from any combination of detectors, such as in the event of equipment failure.

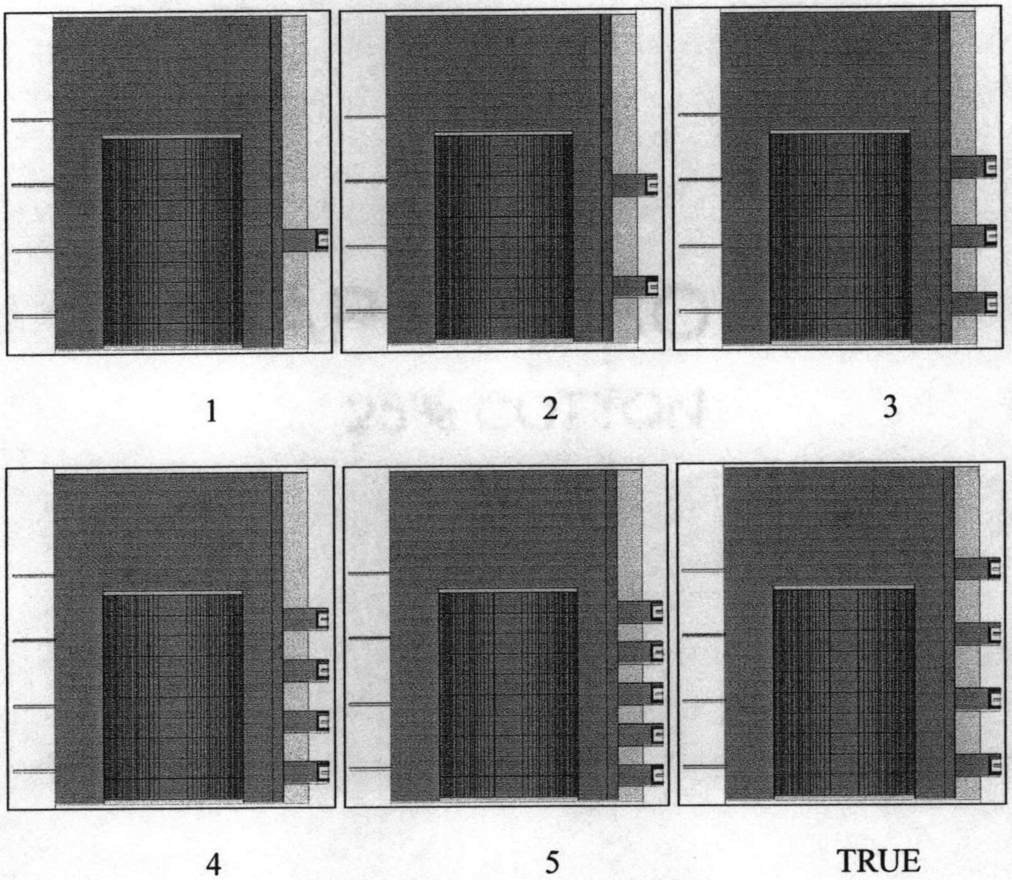

Figure 4. 1,2,3,4 and 5 detector systems.

Given that MDA is a function of efficiency, the study must take into account the effect of different waste drum fill materials that, through attenuation, reduce the number of photons reaching the detector. Three materials are chosen for this study: normal (atmospheric) air, water, and water at half density. Each geometry must then be analyzed with each fill material. While water is perhaps not the most likely nor realistic fill material, especially in the case of an artificial half-density, the fill materials are chosen to represent a range of electron densities possibly encountered in the drums. When simulating photon attenuation, it is this electron density, not the chemical composition, of the material that affects results. Choosing these chemically simple materials keeps the MCNP coding complexity to a minimum.

Running simulations for such an extensive range of geometries and fill materials is computationally expensive. This burden is reduced by only running the entire set of 6 geometries for one fill material. 1, 3, and 5 detector geometries can then be simulated with the remaining two fill materials, and the remaining data interpolated based on the pattern established with the first fill material.

STOCHASTIC SOURCE SIMULATION

The primary obstacle in calculating MDA values for a GEA system is the stochastic nature of the source distribution. The efficiency of detectors in any geometry will vary depending on how the sources are distributed in the drum. The approach taken in this study is to simulate 20 random source distributions to provide a spectrum of efficiencies for each geometry and fill combination. MCNP accommodates multiple source positions easily by letting the user define emission probabilities at each point. The problem then lies in randomly assigning the number of sources and position of each source for each simulation of a given geometry. This problem takes on greater importance with the large number of iterations needed.

The solution chosen for this problem is the division of the drum interior into geometrical cells, or volumetric divisions, each being a potential volume source location. The rotation of the drum during the detection period dictates that each possible cell be a cylindrical shell whose inner and outer radius define the radial distance to inner and outer edges of the source. These concentric cylindrical shells defining the drum interior are then vertically divided into 10 equal-height tiers.

The size of the cylindrical shells representing sources during rotation must satisfy two criteria. First, the shells must be on the same size scale as realistic source sizes encountered in the waste drums. This condition maintains applicability of the results to the actual GEA system. Second, the shells must be defined in such a way that any shell chosen at random has equal probability of containing a source.

One approach would be to divide the interior such that all shells have equal radial thickness. In this method, the shells would contain increasing volumes at further distances from the center. Shells toward the exterior of the drum would thus have a higher probability of containing a source, but the particle emissions would be spread over a larger volume. Source location would then be a function of a randomly chosen vertical tier, and then a randomly chosen shell on that tier whose probability of containing a source is proportional to the mean radius of the shell, squared. This position sampling would be a complex multi-step process than single random number generation, and is perhaps a topic for future studies.

An alternate method, the one chosen for this study, requires that the area, not the radial distance, between the circles defining the inner and outer edges of the shell be equal, i.e. each shell in the 3-dimensional tier has equal volume. The probability of a shell containing a source is then identical for all shell radial locations and tier heights. Source position assignment becomes a random number (integer) generation, with every allowable number referring to a unique shell.

For this study, the drum interior was divided into 10 tiers of 25 concentric shells each (**Figure 5**). Therefore, each shell has 1/250 of the total volume. Given that a 55 gallon drum has an interior radius of 28.4 cm giving a circular area of 2,536 cm^2, the radii of each shell's exterior edge are at values (r)

$$\boxed{r = \sqrt{\frac{n * (101.47)}{\pi}}} \qquad \text{where } n \in \{1, 2, 3, \ldots, 25\}$$

Once a source has been assigned to a shell during a particular MCNP iteration, proper position sampling within the shell must be maintained. The source is constantly rotating around the centerline of the drum, the distant part of the source traveling linearly faster than the near part of the source. This once again raises the problem that MCNP must sample a particle starting location that varies with distance from the center of the drum. However, this time the probability is proportional to the circumference of the circle scribed by the rotation. MCNP automatically accounts for this with the definition of a cylindrical source distribution.

The question may be raised as to why this process wouldn't also solve the problems of the first, equal-radial-change method of drum definition. The difference lies in that the first method could be used to determine which shells have a source. In this case, shells containing sources are already chosen. The goal is now to choose a particle starting position within that shell. All locations within the shell are now "allowable" starting locations for particles from that source without discrete changes in probability such as between concentric shells.

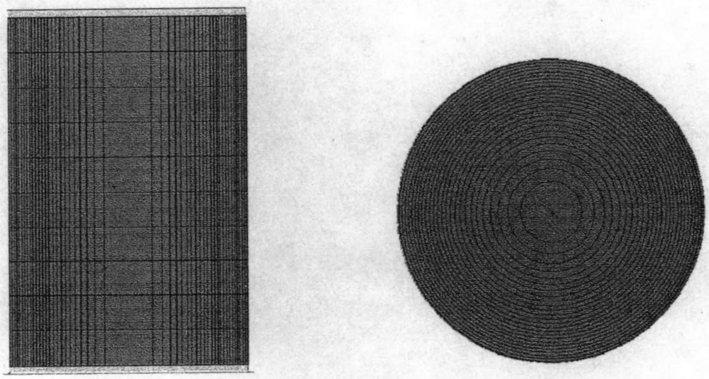

Figure 5. Drum vertical divisions and radial divisions.

Given this division of the drum interior, a stochastically distributed source becomes a matter of random number generation and MCNP input file modification to reflect the chosen source shells. This was accomplished through the development of a program external to MCNP (written in C programming language) that randomly chooses a number of sources (between 1 and 20), then randomly generates a geometrical cell (shell) location number for each. The code then generates the MCNP input file accordingly. Each execution of this program thus generates a MCNP input file with a unique stochastically distributed source.

For each input file, i.e. each unique stochastic source definition, the particle generation location sampling proceeds as follows: For each particle to be born, MCNP randomly chooses one of the cells that the external code has designated as containing a source. A particle genesis position is chosen anywhere within the drum according to the cylindrical source definition and its associated probabilities. However, if the randomly chosen position is not within the chosen cell, it is rejected, and MCNP tries again. The consequence of this is that each cell only contains 0.4% of the drum interior volume, therefore on average 250 particles are generated before one of them is accepted for simulation.

Computing time associated with such an inefficient sampling process is massive. As a solution, fewer particle histories may be simulated. This has the direct effect of raising the relative error in each tally. However MNCP affords a solution. Normally, variance reduction techniques are not permitted with either an F8 pulse height tally or cell source restriction. The single exception to this is directional biasing of the particles once they have been born (Breismeister, 1997).

Considerable computing time is saved by restricting MCNP to only tracking particles headed in the 2-π solid angle toward the detector wall. Radioactive sources emit particles isotropically; meaning that half the particles would actually have been emitted in this forward direction. To account for this, the final tally is automatically divided by two, giving the same result as if particles had been tracked in all 4-π steradian emission directions.

A Unix script runs through 20 iterations of this file generation and processing by MCNP for each geometry-fill combination. Each input and output file is uniquely identified and saved for later reference. The result is a spectrum of 20 efficiency calculations for each detector geometry and for each fill material, from which an average efficiency for each combination can then be derived.

RESULTS

EFFICIENCY AND SPECTRUM NORMALITY

MCNP pulse height tallies record energy depositions in each cell of interest into user-defined energy bins corresponding to counts in multi-channel-analyzer channels of actual radiation detector systems. Channel resolution is therefore an easily programmed value. However, unlike actual radiation detectors, MCNP measurements are exact in that the exact energy loss in each event is known;

MCNP spectrum peaks have no width. Summing the counts under a given peak is consequently not an issue.

Additionally, modeling a mono-energetic photon source eliminates the need for subtracting Compton spectrum background counts from a photopeak count. The photopeak stands clearly by itself approximately 0.253 MeV above the Compton edge (**Figure 6**).

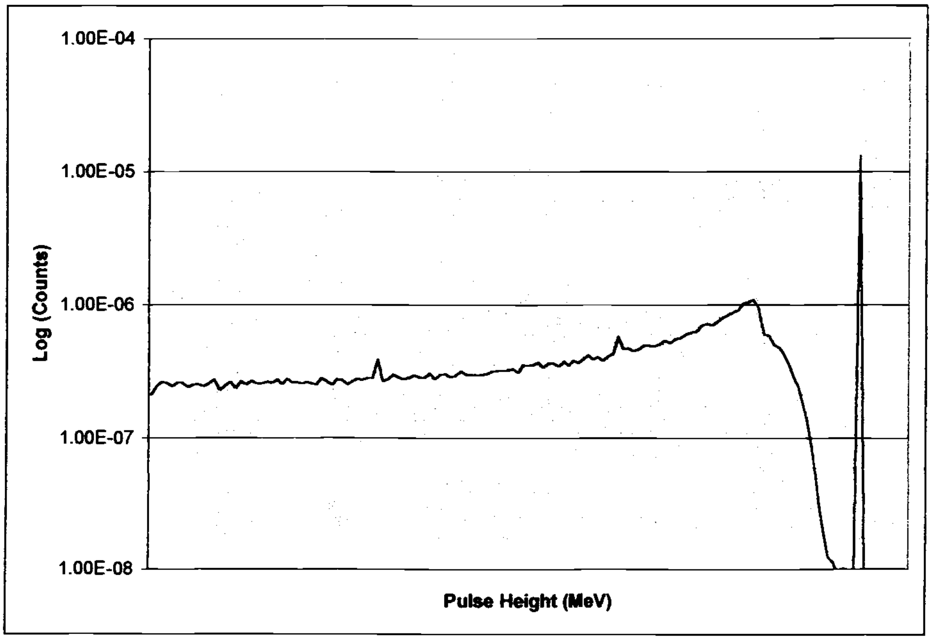

Figure 6. Example MCNP spectrum showing separation of lone photopeak.

Tallies are recorded separately for each cell, i.e. each detector, specified. Total efficiency for a system geometry is the sum of the efficiencies of the individual detectors in the system. Assuming that the relative errors are small enough to indicate valid Monte Carlo measurements (less than 10%), it is later shown in this study that tracking and propagating the errors at this point is unnecessary.

The spectrum of efficiencies of a given geometry is expected to follow an exponential shape similar to a Normal distribution. This can be easily visualized: In a system with a single detector centered vertically beside the drum, randomly placed sources will yield much lower efficiencies near the top and bottom extremities of the drum than sources centered in the drum and thus in front of the detector. The detector efficiency from each source changes exponentially with the vertical offset of the source. Plotting the efficiency for a source at a given location in the drum against the height of that location will yield an exponential curve fitted vertically in the drum (**Figure 7**). This is due to the physics of the system rather than a true statistical fluctuation of each value. However, the exponential shape can be analyzed by fitting the values to a statistical normal distribution. Such an arbitrary fitting was used in this study.

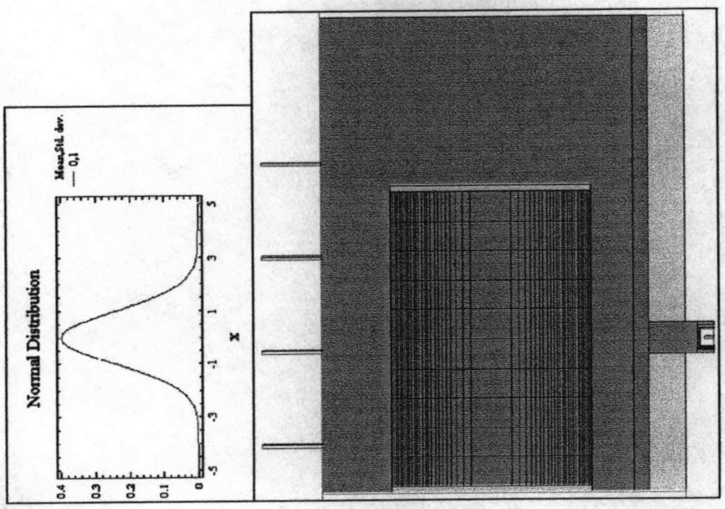

Figure 7. Drum source distribution profile mimics a normal distribution shape.

As a check of this concept, the normality of an efficiency spectrum is verified visually with a statistical Q-Q plot, and then with multiple normality tests by statistical analysis software. For example, below are the normality analysis results for 20 simulations of the 1-detector geometry with an air-filled drum:

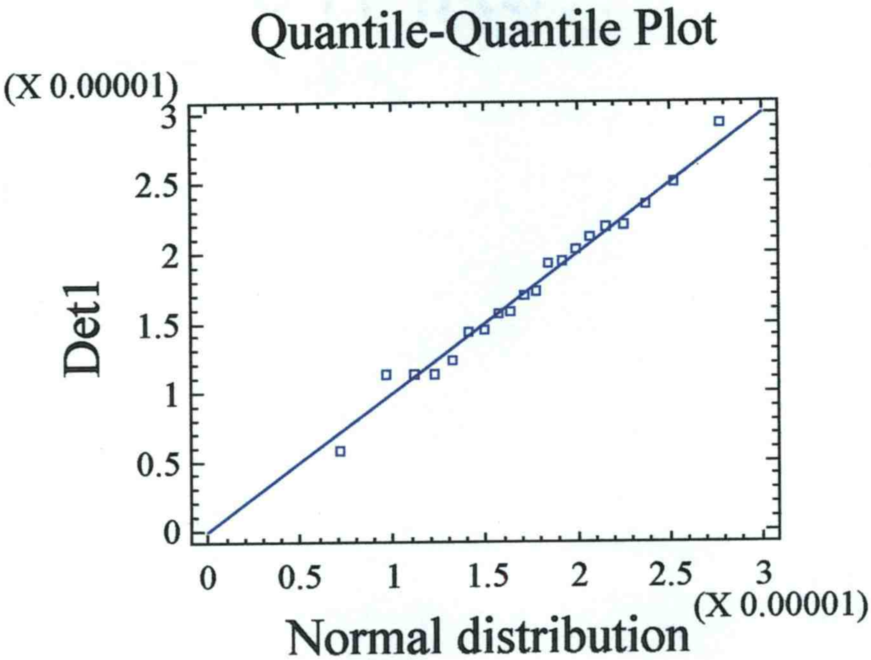

Figure 8. Q-Q plot of data fitted to a normal distribution.

Mean	1.74E-5
Standard Deviation	5.62E-6

Test	Tests for:	Result	P-Value
Chi-Square goodness-of-fit	Number of observations in each of 13 classes versus expected	4.7	0.910
Shapiro-Wilks W statistic	Quantiles of the data versus those of the fitted normal distribution	0.988	0.989
Z Score for Skewness	Lack of symmetry	0.078	0.937
Z Score for Kurtosis	Peak which is either flatter or sharper than a normal distribution	0.154	0.877

Table 1. Testing an efficiency spectrum for normality.

Since the lowest P-value is 0.877, we can not reject the hypothesis that the one-detector geometry comes from a normal distribution with 90% or higher confidence.

In several geometry analyses, the Chi-Square goodness-of-fit test yielded a P-Value below 0.10, leading the analysis software to conclude the data was not from a normal distribution. However, P-Values for the other 3 tests in each case were well above the 90% decision level. This raises the question of how data that passes the majority of analyses can fail the Chi-Square test. A likely answer comes from examining what the test is based on. A Chi-Square goodness-of-fit test divides the values into 13 categories, and then compares how many results are in each category with what would be expected for a normal distribution. A limiting factor in the MCNP data is that only 20 values are available for each geometry due to constraints on computing time. Twenty values divided into 13 categories is obviously a limited analysis. It is expected that additional simulations of each geometry would fill-in sparse areas in the distribution, yielding better results for the Chi-Square test.

Normality indicates that an arithmetic mean (x) is a good representative value of the spectrum and that 95% of the efficiency values will lie above [(x)-(1.65 standard deviations)]. The standard deviation from the mean is easily calculated from the data. Calculations in this report are based on this mean spectrum efficiency as well as the [(x)-1.65σ] conservative 95% confidence efficiency, denoted 95%C, above which 95% of the efficiency values will lie. Fitting the data to a normal curve additionally eliminates the need for propagating the error from each of the 20 individual MCNP detector tallies in a spectrum. Rather, the compounded error is accounted for by this fit distribution.

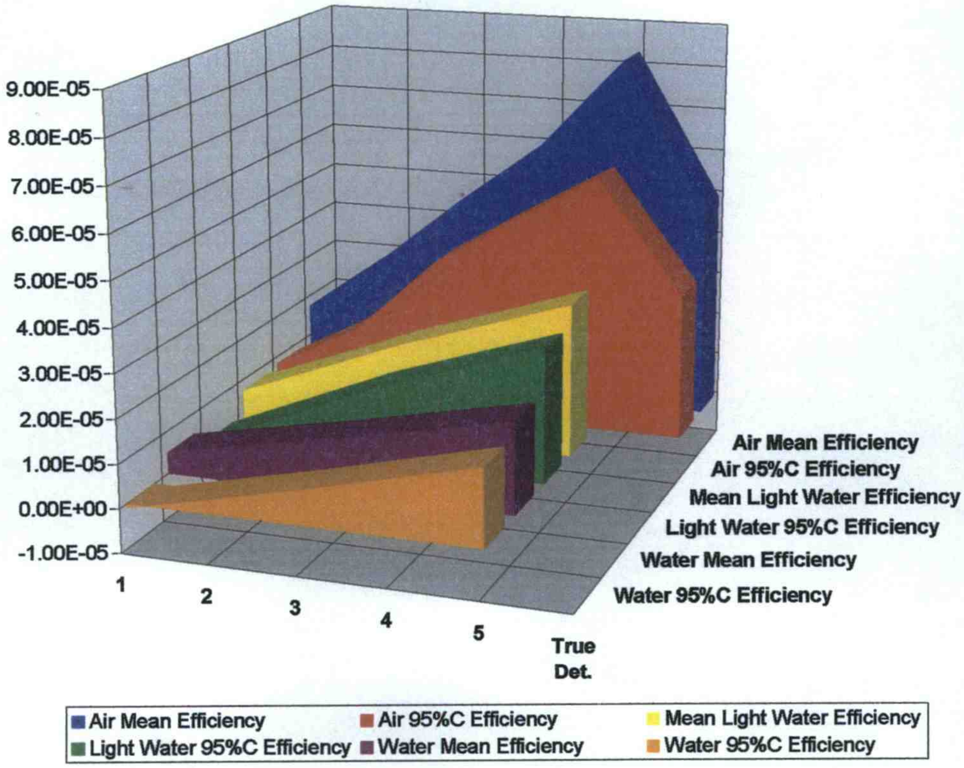

Figure 9. Efficiency results from MCNP simulations.

The next information necessary for an MDA calculation is the background count rate for the system. Background counts are very much a property of individual detectors. The goal of this study is to evaluate the MDA of general system designs and geometries, not to characterize an individual detector. Background counts for each detector could ideally be adapted from actual Fluor Hanford data for detectors in similar positions and treated as constant in the MDA calculations. For example, the background count of a single detector at the vertical midline of the drum is taken as the average of the counts of the actual detectors immediately above and below this position. Total background counts for a system geometry would then be taken as the sum of the expected backgrounds for each detector position in that geometry. However, in the time frame of this investigation the background count data were unavailable. A background count of 200 counts in ten minutes per detector was assumed to allow completion of the study. In the future, calculations could be refined with improved background data.

MINIMUM DETECTABLE ACTIVITY

Normal distribution of the efficiency as well as normal distribution of the background counts should cause the MDA values to follow a log-normal distribution, altering the K_α and K_β values. However, variations in efficiency have already been accounted for by selecting specific values, the mean and conservative efficiency, for use in calculations. Additionally, although variation in background counts follows a normal distribution, the relative values of the variation are often small enough compared to the variation in the efficiency that the shift from a normal to a log-normal distribution would be minimal.

With this in mind, there is enough information to calculate MDA values for each of the 6 detector geometries for each of three fill materials. Again denoting "Mean" as values uncorrected for statistical uncertainty, and "95%C" for the conservative 95% confidence corrected values:

	Air-Fill		Light-Water Fill		Water-Fill	
Geometry	**Mean MDA**	**95%C MDA**	**Mean MDA**	**95%C MDA**	**Mean MDA**	**95%C MDA**
1	0.17	0.36	0.41	2.40	0.58	-3.09
2	0.13	0.23	0.28	0.45	0.47	1.20
3	0.11	0.14	0.23	0.29	0.40	0.65
4	0.10	0.12	0.21	0.25	0.35	0.46
5	0.08	0.11	0.19	0.22	0.32	0.38
True (4)	0.12	0.18				
				All Activities in uCi		

Table 2. MDA Results based on mean and 95% lower confidence limit efficiencies.

It is interesting to note the negative MDA for the case of the 95% confidence water filled 1-detector situation. This is due to the efficiency being lower from attenuation through the water, coupled with a higher standard deviation among the values. Calculating 1.65 standard deviations below the mean gives a negative efficiency in this case, and consequently a negative MDA. Obviously negative values are not possible, but this result was retained to maintain the integrity of the data.

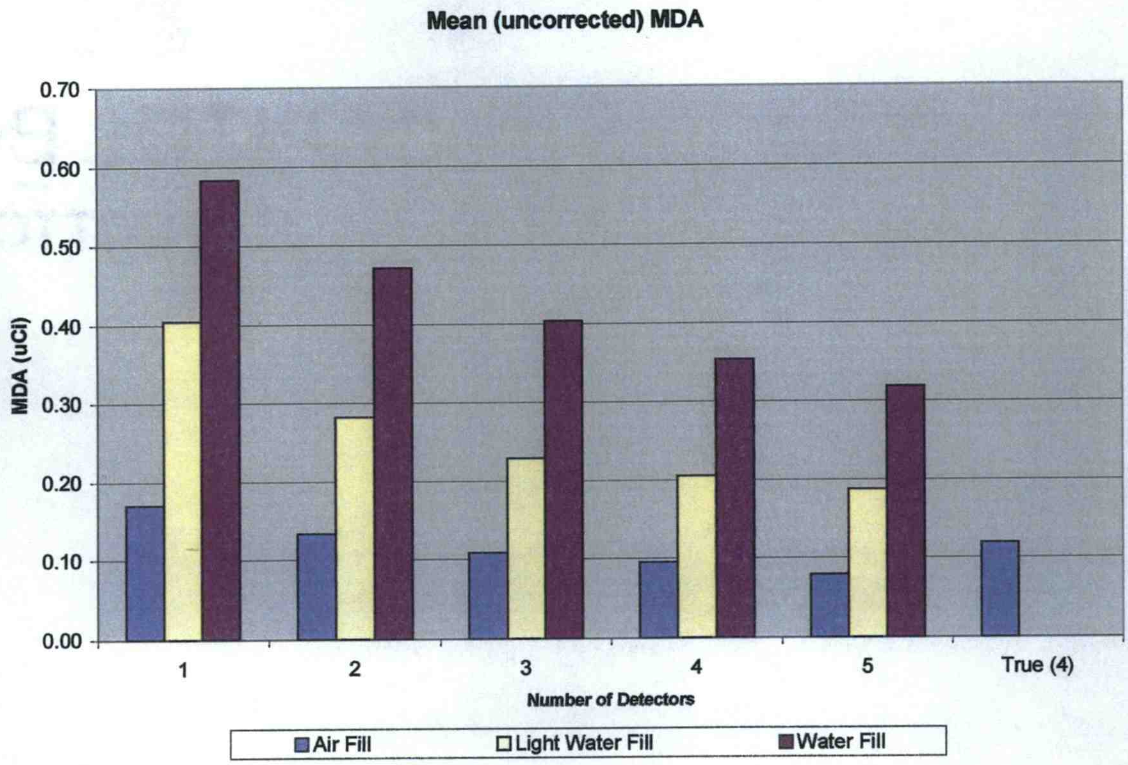

Figure 10. Calculated MDA based on spectrum mean efficiencies.

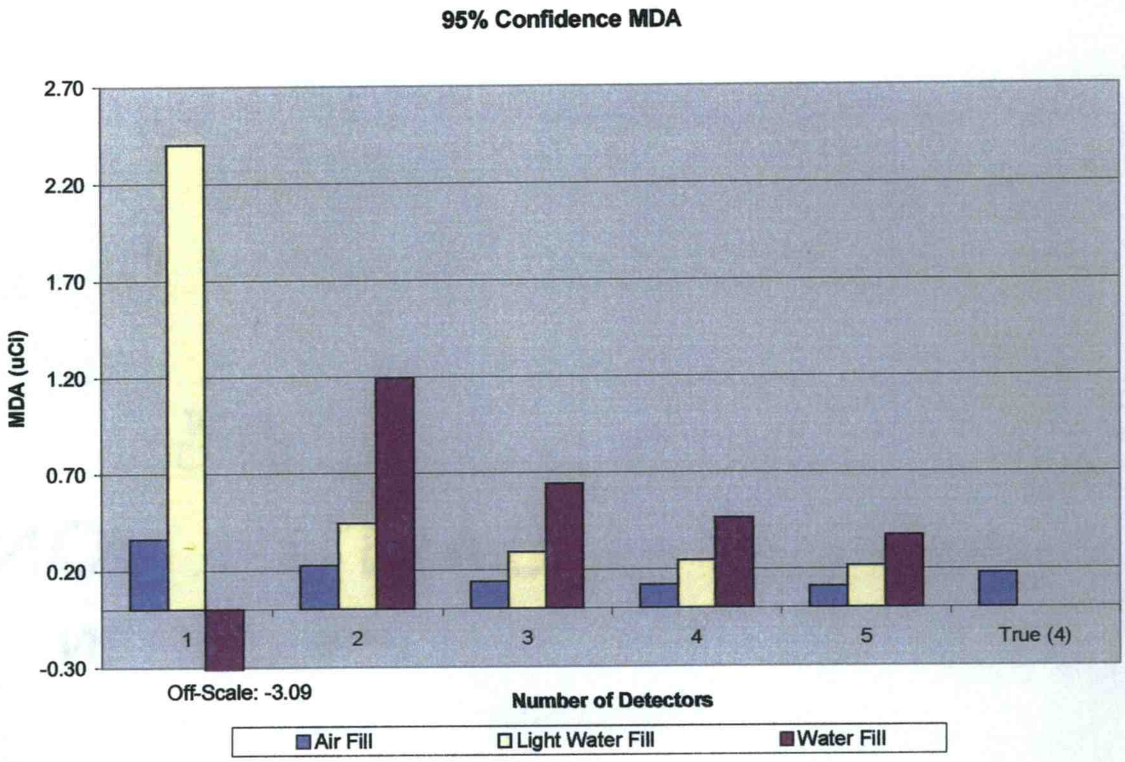

Figure 11. Calculated MDA based on spectrum lower 95% confidence limit efficiencies.

A useful check of the results is to compare the decrease, or benefit, in MDA from each additional detector. In reality, additional detectors will not each add the same efficiency. I.e., a third detector will not add as much as the second, and a fourth will not add as much as the third. This is due to the finite size of the waste drum, and additional detectors being nearer the ends, thus having decreasing solid angles of source to detect.

However, a useful approximation can be made by noting that, in the experimental data, the efficiency contribution from each additional detector is near constant.

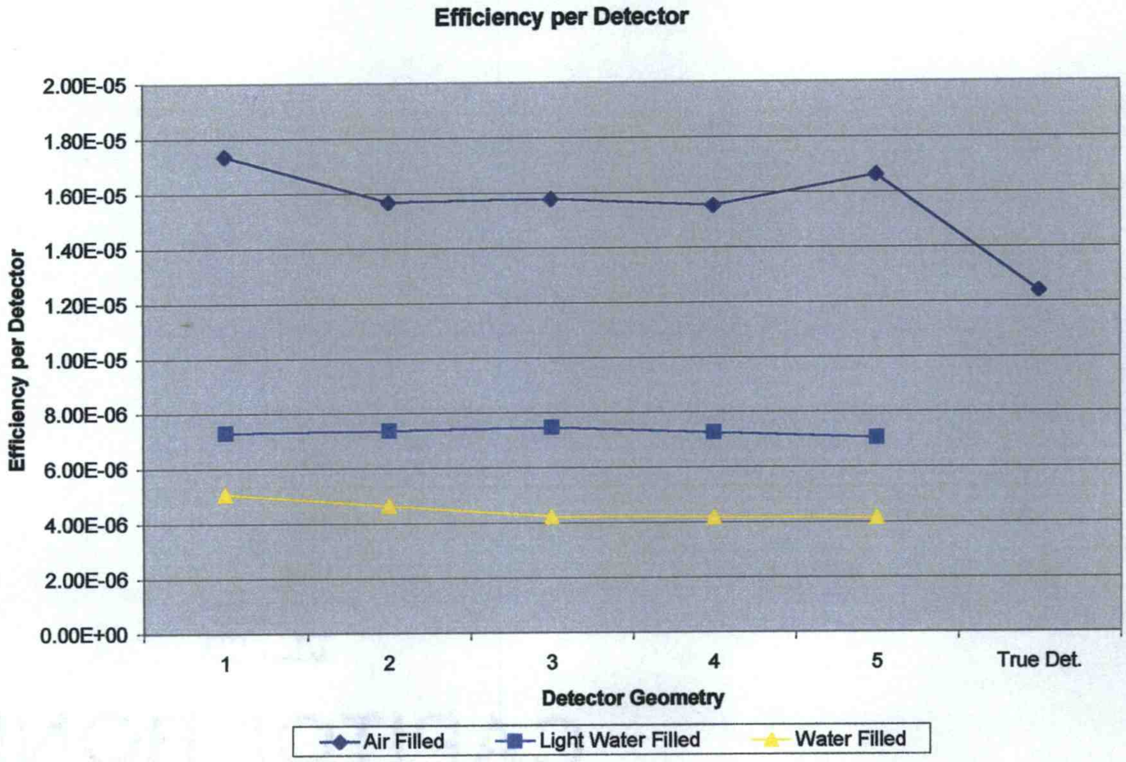

Figure 12. Mean efficiency per detector remains stable.

Thus, in theory, each geometry's MDA should equal the original, one-detector MDA, times a modifying factor. Given that background count rate and efficiency are linear functions of the number (n) of detectors, MDA of a given geometry (MDA_n) versus the one-detector value (MDA_1) is:

$$\boxed{MDA_n = \frac{4.65 * \sqrt{n * N_b}}{n * (eff) * t} = MDA_1 * \left(\frac{\sqrt{n}}{n}\right) = MDA_1 * \left(\frac{1}{\sqrt{n}}\right)}$$

where the original MDA formula has been altered by multiplying both the background count value and efficiency value by the number of detectors in the system. MDA of a given geometry should theoretically be equal to the one-detector MDA times the factor $\left(\frac{1}{\sqrt{n}}\right)$, giving an improvement of $\left[1-\left(\frac{1}{\sqrt{n}}\right)\right] * 100\%$. Additionally, the improvement of each subsequent detector over the previous is $\left[\left(\frac{1}{\sqrt{n}}\right) / \left(\frac{1}{\sqrt{n-1}}\right)\right] = \left(\frac{\sqrt{n-1}}{\sqrt{n}}\right)$, giving an improvement of $\left[1-\left(\frac{\sqrt{n-1}}{\sqrt{n}}\right)\right] * 100\%$. Both of these relations confirm the intuitive idea of diminishing returns for installing additional detectors.

Given these relationships, the comparison of improvement per detector can now be made in figures 13 and 14:

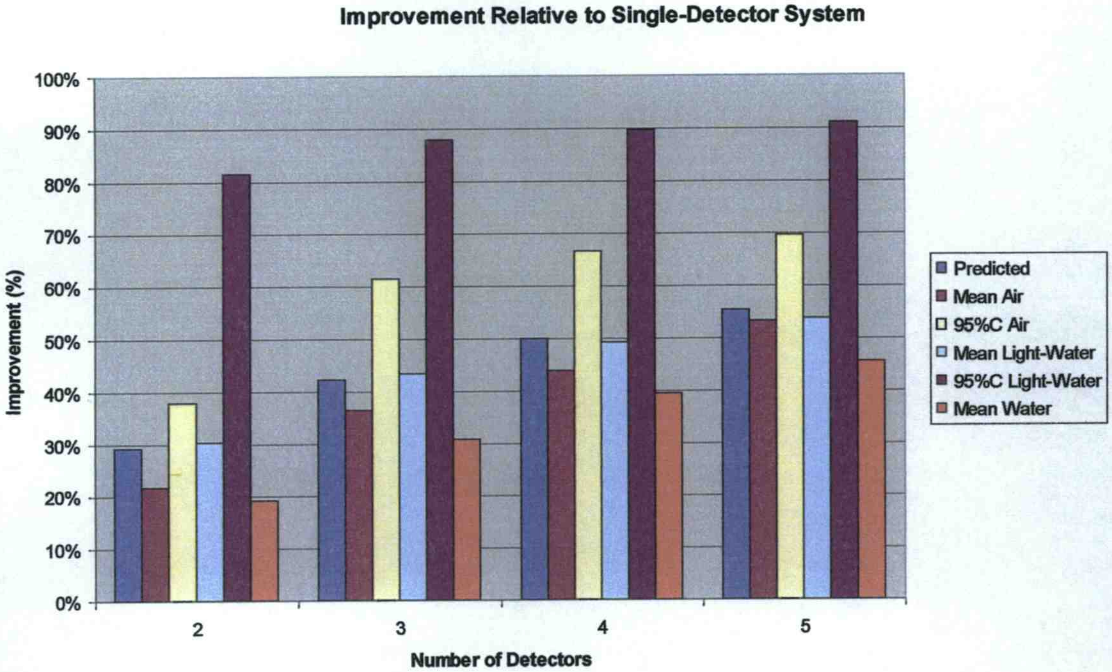

Figure 13. Expected and measured MDA improvement relative to a single detector system.

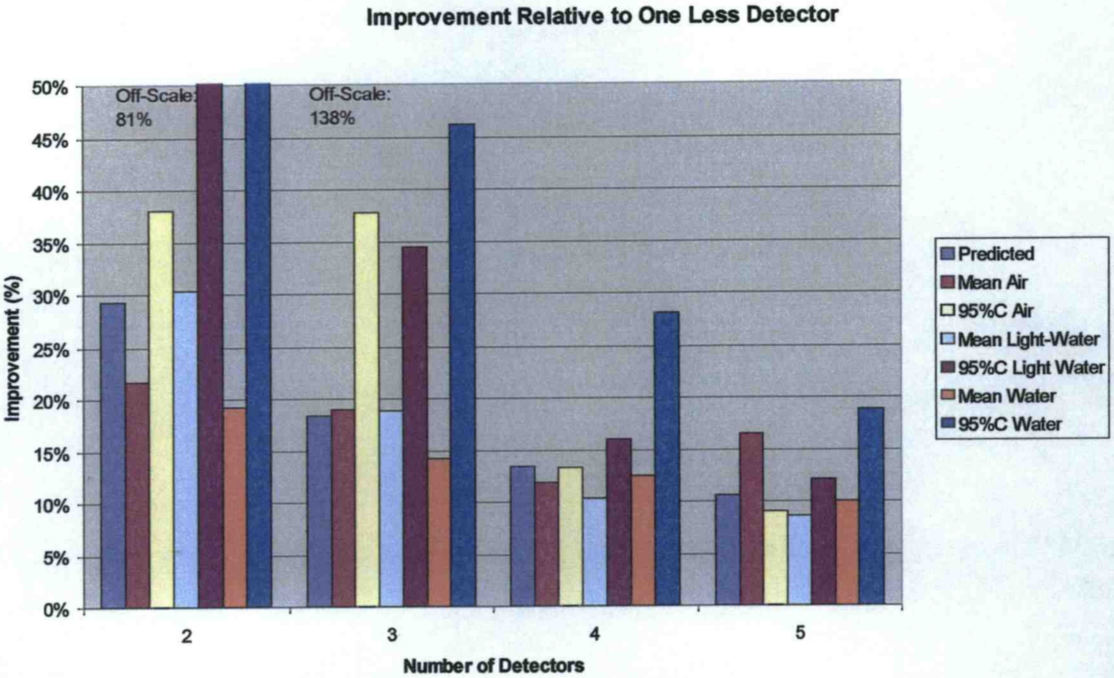

Figure 14. Expected and measured MDA improvement relative to system with one less detector.

As the data demonstrate, the predicted improvement pattern holds true for the mean measured efficiencies of each geometry, but is less reliable for the 95% confidence efficiency levels due to the variable uncertainty of each mean.

FAILURE OF "TRUE" GEOMETRY

To this point, the analysis has been primarily of theoretical GEA geometries with increasing numbers of evenly spaced detectors along the height of the waste drum. As mentioned before, the actual geometry in use at the WRAP facility is four detectors placed such that either the top or bottom detector overshoots the waste drum. In this section, an investigation is made of this "true" geometry MDA, and the effect of detector failure. Only the air-filled drum is modeled in the interest of reducing computing time. Using the previous sections' data as a model, it is assumed that cases of other fill materials would follow the same pattern.

The method of calculating MDA is the same as before. This time, however, counts from the failed detector(s) in each case were excluded from the total efficiency in each MCNP iteration. The spectrum of efficiencies were again used to find a mean, standard deviation, and conservative 95% confidence value for each geometry-fill combination. Denoting each detector as number 1,2,3 or 4 counting from the top, the results were as follows in **Table 3** and **Figure 15**:

Situation	Mean MDA (uCi)	95%C MDA (uCi)
No-Fail	0.12	0.18
1-Fail	0.11	0.16
2-Fail	0.16	0.40
3-Fail	0.16	0.30
4-Fail	0.14	0.22
1,2-Fail	0.14	0.44
1,3-Fail	0.14	0.26
1,4-Fail	0.12	0.19
2,3-Fail	0.29	6.89
2,4-Fail	0.22	0.60
3,4-Fail	0.21	0.68

Table 3. MDA in event of single or multiple detector failures.

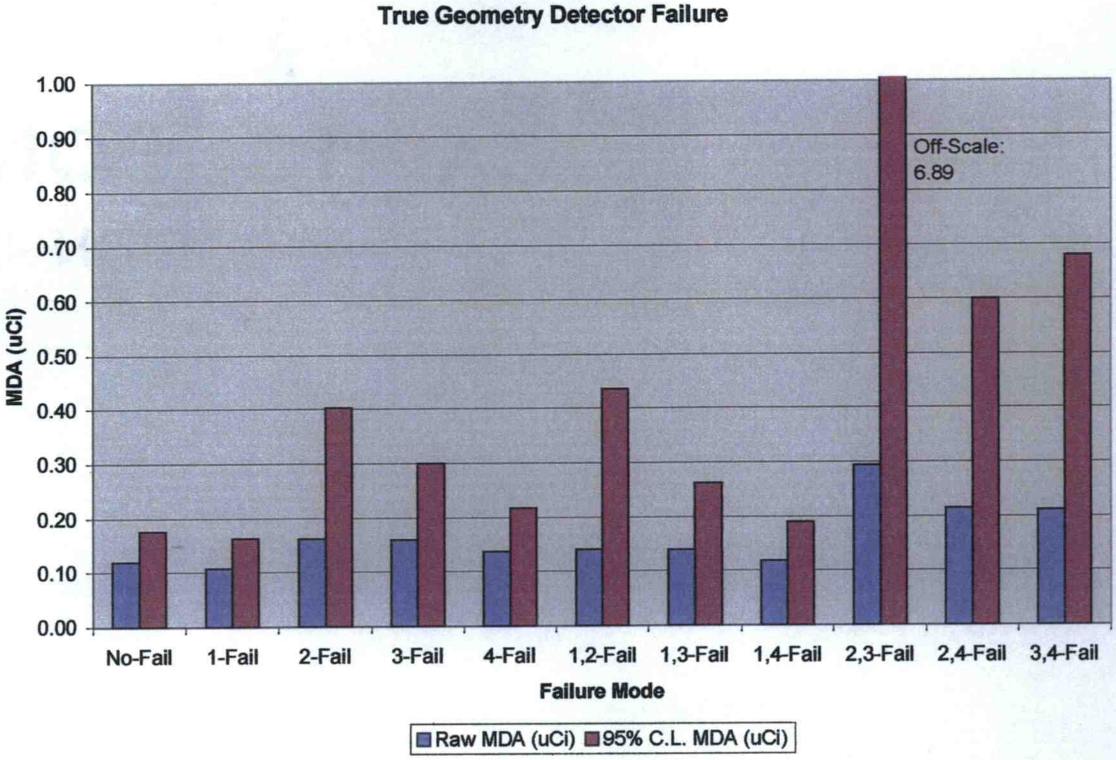

Figure 15. MDA for actual system design in the event of single or multiple detector failure.

As would be expected, the system has the lowest efficiency and highest MDA when detector numbers 2 and 3, the two most centered on the drum, fail. Minimum detectable activity based on the mean efficiency values follow what would be expected for each situation. However, the large standard deviations used to calculate the 95% confidence efficiencies cause wild fluctuations in the MDAs. Most notable is the case of the 95% confidence MDA for detectors 2 and 3 failing. Efficiency in this system is extremely low, which also causes larger error in the MCNP tally value. This causes the 95% confidence efficiency to be extremely low compared to the mean efficiency, largely increasing the 95% confidence MDA over the mean MDA.

ERROR PROPAGATION

The idea of error propagation from each variable in the MDA formula is complex. The two K values are arbitrarily chosen thresholds, and thus have no associated error. Likewise, measurement time can be recorded with such precision that there is no error contribution. The formula itself is designed to account for fluctuation in both the background and source decay values. In this manner, error propagation from these values has already been accounted for by designing the formula to be 95% conservative with respect to each.

One potential shortfall of this version of the MDA formula is that the background normal distribution is assumed to be centered on the single observed value. If the background value is well known, such as through extended counting times or multiple measurements, then the "2" multiplier under the radical disappears, and the MDA is reduced by a factor of the square root of two, or 1.41.

The only remaining variable that introduces error into the MDA calculations of this study is the error of the efficiency value itself. The relationship of MDA to efficiency is inversely linear. For example: if the MCNP predicted efficiency is double the actual value, the reported MDA value will be half the actual value. This study attempted to account for potential errors in the efficiency values by reporting both the MDA calculated from the mean efficiency, and the MDA calculated from the 95% conservatively low efficiency value. A calculation could also have been made from the 95% conservatively high efficiency value, giving the lower limit of MDA. However, the goal behind defining an MDA is to set a sufficiently high threshold that any activity above this value will be recorded at least 95% of the time. Calculating a conservatively low MDA value serves no functional purpose. This being considered, error propagation of the efficiency values has then already been performed by calculating the 95% conservatively high MDA values.

PROBLEM AREAS, FUTURE STUDIES

The rotation of a waste drum during measurement, while simplifying the modeling, also introduces error and a topic for further study. As the drum rotates the source through 360 degrees, it leaves a continuous path of source positions. Source emission probability from each position is a function of the time spent in that position during the counting period. The cylindrical shell model of source regions used in this study only holds true if the drum is in exactly the same rotational position at the start and end of the counting time. Otherwise, any incomplete rotation loop leaves an overlap, and thus a non-uniform probability of emission around the shell.

One important simplification if this is to be modeled is that, in the case of long-lived isotopes, emission probability is deposited uniformly and equally by each rotation. Consequently, each rotation brings the probability to an integer multiple of that from a single rotation. Overlapping regions are therefore simple to model. For example, if the overlapping region created by an incomplete rotation is one-third, or 120 degrees, after N complete rotations, then the relative additional source probability in that region is $(N+(1/3))/(N)$. It is this relationship that allowed overlap to be neglected in this study. After a large number of rotations, such as an extended counting time, the relative probability approaches one, and the error introduced is minimal.

A second area of possible future study is the inclusion of random region volume, isotopes, activities, and fill material in each source region. This would introduce heterogeneous fill material and true source variability, and would inherently be a better model of the actual waste drum configurations. However, this would be a massive undertaking, and MCNP is perhaps not the simulation program of choice.

Cylindrical shell modeling of source regions also introduces several other obstacles. Given improved computing time, for which MCNP offers many possible solutions, drum division resolution could be much improved. This would not only offer improved source location possibilities, but would also prevent a region division lying directly in front of a detector, as is the case for the middle of five detectors. It is unknown exactly how much error is introduced by situations such as this, and is a topic needing future study.

The largest and most pressing source of error is insufficient benchmarking of the germanium detector models against known systems and results. As is often discussed in literature, the best results from MCNP are achieved by altering parameters to calibrate to known results rather than faithfully modeling physical geometries. In the course of the initial work for Fluor Hanford, some benchmarking was possible, but not nearly enough to guarantee true detector efficiency measurements. Much more time and experimental data from various situations would be needed. It is for this reason that the focus of this paper is on the method rather than absolute values. If, in the future, more benchmarking is possible, it would be relatively simple to incorporate the changes into these MCNP simulations and re-calculate the MDA values.

CONCLUSION

The Canberra GEA vaults in use at the Fluor Hanford WRAP Facility are important non-destructive analysis tools for characterization of trans-uranic waste drums. Minimum detectable activity of these systems is a characteristic in ensuring the measured results, however the stochastic distribution of the sources in the waste drums makes this difficult. This study demonstrated a technique to estimate MDA for stochastically distributed sources using MCNP Monte Carlo simulations and an external code to randomly assign sources to volumetric regions in the waste drum. Furthermore, alternative GEA designs and drum fill materials were investigated, as well as MDA in the event of detector failure.

In all, this study's technique is an effective way to determine MDA with the adverse condition of stochastically distributed sources. Other approaches are certainly possible, but the evidence suggests that this method matches both intuitive expectations as well as patterns predicted by the MDA formula. After additional studies, it may eventually prove an integral part of benchmarking system performance in coordination with physical experiments.

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